

SEQUENTIAL CHANGE-POINT DETECTION BASED ON NEAREST NEIGHBORS

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We propose a new framework for the detection of change points in online, sequential data analysis. The approach utilizes nearest neighbor information and can be applied to sequences of multivariate observations or non-Euclidean data objects, such as network data. Different stopping rules are explored, and one specific rule is recommended due to its desirable properties. An accurate analytic approximation of the average run length is derived for the recommended rule, making it an easy off-the-shelf approach for real multivariate/object sequential data monitoring applications. Simulations reveal that the new approach has better performance than existing approaches for high dimensional data. The new approach is illustrated on two real datasets: Detecting global structural change in a social network and detecting change in word usage.

1. Introduction. Sequential change-point models are widely used in many fields to detect events of interest as data are generated. One of its early applications is in quality control where a summary statistic reflecting a manufacture process is monitored over time. When the statistic begins to exhibit values that are unlikely to be achieved by random fluctuations, there is a high probability that something went wrong and an investigation is needed. Therefore, it is important to detect the change point, the time when the event of interest happens, as soon as possible if it occurs, while keeping the false discovery rate low; refer to monographs [Wald \(1973\)](#), [Siegmund \(1985\)](#) and [Tartakovsky, Nikiforov and Basseville \(2014\)](#) for more background information.

Sequential change-point detection has been extensively studied for univariate data, that is, for data where the observations are scalar at each time point. However, many recent applications involve the detection of change points over a sequence of multivariate, or even non-Euclidean, observations. Following are some motivating examples.

Multiple sensor framework: In a sensor network, hundreds or thousands of sensors are deployed to detect events of interest. For example, hundreds of monitors are placed worldwide to detect solar flares, which are large energy releases by the Sun that can affect Earth's ionosphere and disrupt long-range radio communication ([Kappenman, 2012](#); [Qu et al., 2005](#)). Often, the structure of the sensor network can be used to boost the power of the detection. Then, each observation can be viewed as a vector with some structures among its elements that reflect the spacial information of the sensors.

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Social network evolution: Technological advances provide us with rich resources of social network data, such as networks constructed by Facebook friendship relations, email communications, phone calls, or online chat records. The detection of abrupt events, such as shifts in network connectivity, dissociation of communities, or formation of new communities, can be formulated as a change-point problem. Here, the observation at each time point is a graphical encoding of the network.

Epidemic disease outbreak: It is important to detect the emergence of new infectious diseases as early as possible to prevent their spreadings. In United States, the current practice is that the Center for Disease Control gathers data from hospitals and then integrates information together to tell if there is an outbreak. This process usually takes weeks to draw conclusions. Researchers have tried to incorporate other information, such as online searches on disease related topics and climate information, which had success in shortening the prediction lag time for flu outbreaks (Yang, Lipsitch and Shaman, 2015; Yang, Santillana and Kou, 2015). It can be foreseen that, in the future, information from multiple sources will be used to predict disease outbreaks. Then, each observation can be quite complicated and may include hospital admission rates, online search frequencies on related topics, personal posts on related symptoms, and whether information.

Image analysis: Image data are collected over time in many areas. It is of tremendous interest to automatically detect abrupt events, such as security breaches from surveillance videos or extreme weather conditions, e.g., storms, from climatology. In these applications, the data at each time point is the digital encoding of an image.

In all of these examples, the problem can be formulated in the following way: We denote the data sequence by $\{\mathbf{Y}_i\}, i = 1, 2, \dots, n, \dots$, indexed by time or some other meaningful orderings. Here, \mathbf{Y}_i 's can be vectors, networks, or images. The sequence is identically distributed as F_0 until a time τ the distribution changes abruptly to F_1 :

$$\begin{aligned}\mathbf{Y}_i &\sim F_0, & i = 1, \dots, \tau - 1, \\ \mathbf{Y}_i &\sim F_1, & i = \tau, \tau + 1, \dots,\end{aligned}$$

where F_0 and F_1 are two different probability measures.

There is a burst of works recently on the change-point detection in multiple sequences where the sequences are assumed to be independent, such as in multiple sensor framework where the sensors are assumed to be independent. These works also in general assume the observations over time are independent. Some nice algorithms and theorems have been developed under these assumptions. For example, Tartakovsky and Veeravalli (2008) and Mei (2010) studied statistics that sum signals over all streams with further assumptions that the density functions before and after the change are known and the change happens to all streams at the same time. Xie and Siegmund (2013) and Chan and Walther (2015) allow the change only happen to a subset of the data streams under the assumption that F_0 and F_1 are multivariate normal distributions with identity covariance. The latter paper

also studied the optimality of several statistics. These statistics are useful if the assumptions under which the statistic was developed hold for the data. However, in many applications, it would be too stringent to assume that all data streams are independent.

To another end, the change-point detection problem for dynamic network data is gaining more and more attentions. A number of works have been done if the networks are generated in some specific ways. For example, [Heard et al. \(2010\)](#) developed Bayesian methods by modeling each pair of nodes independently and they modeled the communications between nodes over time as a counting process with the increments of the process following a Bayesian probability model. A multinomial extension that relaxed the independence assumption among pairs of nodes was also studied by the authors. [Wang et al. \(2014\)](#) considered the setting that the series of networks are generated by a stochastic block model with the block membership of the vertices fixed across time. They use locality-based scan statistic to find change-point where the connectivity probability matrix varies. Again, these methods are useful if the data do satisfy the assumptions, while these assumptions could be too specific for many applications.

In this paper, we describe a nonparametric framework to approach the problem. This framework can be applied to data in arbitrary dimension and to non-Euclidean data, with a general, analytic formula for false discovery control. The proposed method adopts the idea of making use of similarity graphs, such as nearest neighbors, among the observations in [Chen and Zhang \(2015\)](#).

In the following, we do not impose specific assumptions on F_0 or F_1 . However, we assume the observations over time are independent. When there is weak dependence over time, the graph-based approach could still provide meaningful results for change-point analysis as shown in [Chen and Zhang \(2015\)](#). Also, the independence assumption is a natural starting point for more sophisticated models that consider dependency over time.

[Chen and Zhang \(2015\)](#) studied the problem of *offline* change-point detection, where all observations are completely observed at the time when data analysis is conducted. However, in many applications, it is desirable to detect change-points on the fly. There are both theoretical and computational challenges to extend the method in [Chen and Zhang \(2015\)](#) to the *online* framework. In particular, adding new observations usually changes the similarity structure among existing observations, when the most similar observation for an existing observation may be changed to the newest observation. This makes the theoretical analysis on false discovery control much harder as it requires an analysis of the dynamics of similarity structural change when new observations are added.

In this paper, we consider the similarity structure represented by nearest neighbors (NN). We studied the dynamics in NN updates as new observations are added. It turns out that the characterization of a small number of events, in particular, the updates of mutual NNs and shared NNs, and all three-way interactions among the NN relations, could capture the majority of the dynamics (see Section 5 for details). This makes the task tractable. We can also easily implement the method for real data applications.

The rest of the paper is organized as follows: In Section 2, we briefly review a two-

sample test based on NNs, which is a building block for the change-point analysis. In Section 3, we discuss details of the proposed detection method and three stopping rules. We recommend the use of the stopping rule that relies on recent observations for its desirable properties. In Section 4, we study the updating dynamics of NNs and derive an analytic formula for false discovery control that is accurate for finite samples. In Section 5, we compare the proposed method to parametric methods for multivariate data. We illustrate the proposed method on two real datasets in Section 6. In Section 7, we briefly discuss the choice of the number of nearest neighbors and the performance of the proposed method on gradual changes.

2. A brief review of the two-sample test on k -NN. In this section, we review the two-sample test on k -NN proposed by Schilling (1986) and Henze (1988). Here, k is a fixed integer. Let k -NN be the directed graph with the pooled observations as the nodes and each node points to its first k NNs. It is assumed that the observations are distinct with uniquely defined neighbors. (This happens with probability 1 if \mathbf{Y}_i 's follow continuous multivariate distributions and the Euclidean distance is used.)

Let $\{\mathbf{Y}_1, \dots, \mathbf{Y}_{n_1}\}$ and $\{\mathbf{Y}_{n_1+1}, \dots, \mathbf{Y}_{n_1+n_2}\}$ be random samples from two populations, and let $n = n_1 + n_2$ be the total sample size. For any event x , let $\mathbf{I}(x)$ be the indicator function that takes value 1 if x is true or 0 if otherwise. Let

$$b_{ij} = \mathbf{I}((i \leq n_1, j > n_1) \text{ or } (i > n_1, j \leq n_1)),$$

then b_{ij} is the indicator function that \mathbf{Y}_i and \mathbf{Y}_j belong to different samples. We want to test whether these two population distributions are the same or not. Let

$$A_{ij}^{(r)} = \mathbf{I}(\mathbf{Y}_j \text{ is the } r\text{th nearest neighbor of } \mathbf{Y}_i), \quad A_{ij}^+ = \sum_{r=1}^k A_{ij}^{(r)}.$$

Then A_{ij}^+ is the indicator function that \mathbf{Y}_j is among the first k NNs of \mathbf{Y}_i . We have $A_{ij}^+ \in \{0, 1\}$ and $\sum_{j=1}^n A_{ij}^+ = k, 1 \leq i \leq n$. Then

$$\sum_{i=1}^n \sum_{j=1}^n A_{ij}^+ b_{ij} \equiv \sum_{i=1}^n \sum_{j=1}^n A_{ji}^+ b_{ij}$$

is the number of edges in the k -NN that connect between the two samples.

Expressing in a more symmetric way, we have

$$\sum_{i=1}^n \sum_{j=1}^n (A_{ij}^+ + A_{ji}^+) b_{ij} \tag{2.1}$$

being twice the number of edges in the k -NN that connect between the two samples. Given the observations $\mathbf{Y}_i = \mathbf{y}_i, 1 \leq i \leq n$, the test statistic is

$$\sum_{i=1}^n \sum_{j=1}^n (a_{ij}^+ + a_{ji}^+) b_{ij},$$

where $a_{ij}^+ = \sum_{r=1}^k a_{ij}^{(r)}$ with $a_{ij}^{(r)} = \mathbf{I}(\mathbf{y}_j$ is the r th nearest neighbor of \mathbf{y}_i). In [Schilling \(1986\)](#) and [Henze \(1988\)](#), the authors proposed to reject the null hypothesis of no difference if the test statistic is significantly *smaller* than its expectation under the permutation null distribution. The rationale is that, if the two samples are from the same distribution, they are well mixed and are likely to find their nearest neighbors from the other sample. So if the observations tend to not find nearest neighbors from the other sample, they are from different distributions.

We denote the random variable under the permutation distribution as follows: Let $B_{ij} = b_{\mathbf{P}(i)\mathbf{P}(j)}$ be the indicator function that \mathbf{Y}_i and \mathbf{Y}_j belong to different samples under random permutation. Here, $\mathbf{P}(i)$ is the index of \mathbf{Y}_i under permutation. Let

$$X = \sum_{i=1}^n \sum_{j=1}^n (a_{ij}^+ + a_{ji}^+) B_{ij}. \quad (2.2)$$

Then its expectation and variance are

$$\begin{aligned} \mathbb{E}(X) &= \frac{4k n_1 n_2}{n-1}, \\ \text{Var}(X) &= \frac{4n_1 n_2}{n-1} \left(h(n_1, n_2) \left(\frac{1}{n} \sum_{i,j=1}^n a_{ij}^+ a_{ji}^+ + k - \frac{2k^2}{n-1} \right) \right. \\ &\quad \left. + (1 - h(n_1, n_2)) \left(\frac{1}{n} \sum_{i,j,l=1}^n a_{ji}^+ a_{li}^+ - k^2 \right) \right), \end{aligned}$$

where $h(n_1, n_2) = \frac{4(n_1-1)(n_2-1)}{(n-2)(n-3)}$. It has been shown that

$$\frac{X - \mathbb{E}(X)}{\sqrt{\text{Var}(X)}}$$

converges to the standard normal distribution under the null hypothesis as long as $n_1/n_2 \rightarrow \lambda \in (0, \infty)$ for multivariate data ([Schilling, 1986](#); [Henze, 1988](#)).

3. Sequential change-point detection based on k -NN. We use

$$\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_n, \dots$$

to denote the data sequence, where \mathbf{Y}_n is the observation at time n . In the following, we assume that we have a well defined norm $\|\cdot\|$ on the sample space such that the distance between two observations \mathbf{y}_i and \mathbf{y}_j can be calculated as $d(\mathbf{y}_i, \mathbf{y}_j) = \|\mathbf{y}_i - \mathbf{y}_j\|$. We also assume that the observations are distinct points in the sample space and have uniquely defined nearest neighbors. In the following, k is fixed. The choice of k is briefly discussed in Section 8.

We assume that there are N_0 historical observations with no change point. That is, $\mathbf{Y}_1, \mathbf{Y}_2, \dots, \mathbf{Y}_{N_0}$ follow the same distribution. This can be determined from prior

information or we can use offline change-point detection methods to test whether there is any change point among the first N_0 observations, such as the method in [Chen and Zhang \(2015\)](#). We begin our test from observation $N_0 + 1$.

For any n , $1 \leq i, j \leq n$, let

$$A_{n,ij}^{(r)} = \mathbf{I}(\mathbf{Y}_j \text{ is the } r\text{th NN of } \mathbf{Y}_i \text{ among the first } n \text{ observations}),$$

Then $A_{n,ij}^+ = \sum_{r=1}^k A_{n,ij}^{(r)}$ is the indicator function that \mathbf{Y}_j is one of the first k NNs of \mathbf{Y}_i among the first n observations.

We can perform a two-sample test for each $t \in \{1, \dots, n-1\}$ with one sample being the observations before t and the other sample being the observations between t and n . Define

$$b_{ij}(t, n) = \mathbf{I}((i \leq t, t < j \leq n) \text{ or } (t < i \leq n, j \leq t)),$$

and $B_{ij}(t, n) = b_{\mathbf{P}_n(i)\mathbf{P}_n(j)}(t, n)$, where $\mathbf{P}_n(\cdot)$ is a random permutation among the first n indices. Let

$$R(t, n) = \sum_{i=1}^n \sum_{j=1}^n (A_{n,ij}^+ + A_{n,ji}^+) B_{ij}(t, n).$$

We use \mathbf{y}_i 's to denote the realizations of \mathbf{Y}_i 's, and let

$$Z_{|\mathbf{y}}(t, n) = -\frac{R(t, n) - \mathbf{E}(R(t, n))}{\sqrt{\text{Var}(R(t, n)|\mathbf{y})}}.$$

Note that $\mathbf{E}(R(t, n)|\mathbf{y}) = \mathbf{E}(R(t, n))$.

If a change point $\tau > N_0$ occurs in the sequence, we would expect $Z_{|\mathbf{y}}(t, n)$ to be *large* (notice the negative sign in the standardization) when $n > \tau$ and t close to τ . We can thus define the stopping rule as

$$T_1(b_1) = \inf \left\{ n - N_0 : \left(\max_{n_0 \leq t \leq n-n_0} Z_{|\mathbf{y}}(t, n) \right) > b_1, \ n \geq N_0 \right\}, \quad (3.1)$$

where n_0 is a pre-specified offset, such as 3. Usually, n_0 is set to be small in order to detect the change as soon as possible, while not too small, such as 1, to avoid the high fluctuations at the very ends. Here, b_1 is chosen so that the false discovery rate of this stopping rule is controlled at a pre-specified level.

When τ is large, the above stopping rule would end up with testing whether an early time is a change point for many times, which is unnecessary. To avoid this, we can modify the stopping rule as

$$T_2(b_2) = \inf \left\{ n - N_0 : \left(\max_{n-n_1 \leq t \leq n-n_0} Z_{|\mathbf{y}}(t, n) \right) > b_2, \ n \geq N_0 \right\}, \quad (3.2)$$

where $n_1 > n_0 > 0$ are pre-specified offsets. We can choose n_1 tactically to avoid unnecessary tests and save computation time.

For both T_1 and T_2 , at time n , we find k NNs among the first n observations. This can be problematic when n is large because $Z_{|\mathbf{y}}(t, n)$ is highly left skewed when t/n is small (see Section 3.1). To address this issue, we can further modify the stopping rule as

$$T_3(b_3) = \inf \left\{ n - N_0 : \left(\max_{n-n_1 \leq t \leq n-n_0} Z_{L|\mathbf{y}}(t, n) \right) > b_3, n \geq N_0 \right\}, \quad (3.3)$$

where $Z_{L|\mathbf{y}}(t, n)$ is defined the same as $Z_{|\mathbf{y}}(t, n)$ but only uses the L most recent observations: $\mathbf{Y}_{n-L+1}, \dots, \mathbf{Y}_n$. That is, for $i, j \in n_L \triangleq \{n-L+1, \dots, n\}$, we let

$$A_{n_L, ij}^{(r)} = \mathbf{I}(\mathbf{Y}_j \text{ is the } r\text{th NN of } \mathbf{Y}_i \text{ among observations } \mathbf{Y}_{n-L+1}, \dots, \mathbf{Y}_n),$$

$A_{n_L, ij}^+ = \sum_{r=1}^k A_{n_L, ij}^{(r)}$, and $R_L(t, n) = \sum_{i, j \in n_L} (A_{n_L, ij}^+ + A_{n_L, ji}^+) B_{ij}(t, n_L)$ with $B_{ij}(t, n_L) = b_{\mathbf{P}_{n_L(i)} \mathbf{P}_{n_L(j)}(t)}$, where $\mathbf{P}_{n_L}(\cdot)$ is a random permutation among indices $\{n-L+1, \dots, n\}$. Then let

$$Z_{L|\mathbf{y}}(t, n) = -\frac{R_L(t, n) - \mathbf{E}(R_L(t, n))}{\sqrt{\text{Var}(R_L(t, n)|\mathbf{y})}}.$$

For any n , $Z_{L|\mathbf{y}}(t, n)$ is based on L observations. This overcomes the accumulation of skewness as n grows.

3.1. Comparisons of the three stopping rules. Two key objectives of sequential detection are (i) to detect the change point as soon as possible when it occurs; and (ii) to keep the false discovery rate low. These can be characterized by two quantities: The expected detection delay, $\mathbf{E}_\tau(T - \tau | T > \tau)$, where τ is the change point; and the average run length, $\mathbf{E}_\infty(T)$, the expectation of T when there is no change point, i.e., the change point at infinity.

We use simulations to compare the three stopping rules. We keep their false discovery rates the same and compare their expected detection delays. The simulation setup is as follows: There are $N_0 = 200$ historical observations from the same distribution. We begin our test from $t = 201$. In the simulation, the change point is at $t = 400$, i.e., 200 new observations from the start of the test. Before the change point, the distribution is a d -dimensional Gaussian distribution with mean μ_1 and covariance matrix I_d , $\mathcal{N}_d(\mu_1, I_d)$; after the change, the distribution is $\mathcal{N}_d(\mu_2, I_d)$. Let $\Delta = \|\mu_2 - \mu_1\|_2$ where $\|\cdot\|_2$ is the L_2 norm.

The thresholds b_1, b_2, b_3 are determined so that $\mathbf{P}_\infty(T_i(b_i) < 1,000) = 0.05$, $i = 1, 2, 3$. That is, when there is no change point, the probability of reporting any change point (false discovery) before $t = 1,200$ (1,000 new observations from the starting the the test) is 0.05. Here, \mathbf{P}_∞ denotes the probability under the event that there is no change point. (According to the Poisson heuristic in [Siegmund and Venkatraman \(1995\)](#), this criterion corresponds roughly to $\mathbf{E}_\infty(T_i(b_i)) = 20,000$. We here control directly on false discovery rather than average run length to reduce simulation time.) We are able to obtain the thresholds, b_1, b_2, b_3 , through simulations here because the distribution of the observations is known. We determine the

thresholds through 10,000 Monte Carlo simulations. Other parameters are set to be $n_0 = 3$, $L = 200$ and $n_1 = L - n_0$.

The expected detection delays are estimated based on 1,000 simulation runs. They are calculated as the averages of the lag of the detection time to the true change point when the change point is successfully detected. We define “successful detection” be to detect the change within 100 observations after it occurred because detecting it too later (say after 100 observations) would usually not be useful in practice.

The expected detection delays of the three stopping rules using 1-NN and 3-NN under different magnitudes of the change (Δ) are plotted in Figure 1. We see that the three stopping rules have very similar expected detection delays. The detection delay is clearly shortened when the signal is stronger (Δ larger) and/or when we include slightly more NNs into the test, from 1-NN to 3-NN.

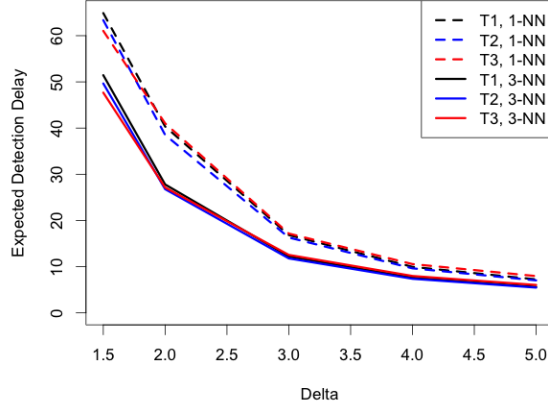


FIG 1. Expected detection delays for the three stopping rules with $k = 1, 3$. The x-axis is the magnitude of the change Δ .

TABLE 1
Failure probabilities for the three stopping rules.

Failure I. Early stops (false discovery)

	T_1	T_2	T_3
1-NN	0.0178	0.0205	0.0107
3-NN	0.0148	0.0183	0.0103

Failure II. Failed to find the change point within 100 observations after the change occurred.

Δ	1-NN			3-NN		
	T_1	T_2	T_3	T_1	T_2	T_3
1.5	0.256	0.233	0.341	0.026	0.022	0.042
2	0.003	0.003	0.021	0	0	0
3	0	0	0	0	0	0
4	0	0	0	0	0	0
5	0	0	0	0	0	0

In some occasions, no change point is detected within 100 observations after the change occurred, and we call this “Failure II”. Table 1, Failure II, shows this failure rate for the three stopping rules under different combinations of parameters. We see that T_1 and T_2 have smaller failure II rates than T_3 , with T_2 the smallest as it removes many redundant tests. However, all failure II rates go to 0 when the signal becomes stronger. When the signal is weak, all failure II rates decrease significantly if we include slightly more NNs into the test, from 1-NN to 3-NN.

In some other occasions, the test reports change points before the true one occurs. We call this “Failure I” (false discovery). They are summarized in Table 1 (Failure I). Since this does not depend on the signal strength (Δ) as it occurs before the change happens, so all occasions are binned according to stopping rules and k . In the simulations, the true change point is at $t = 400$ (200 new observations after the starting of the test). If false discoveries are uniformly distributed along the time, then $P_\infty(T < 200)$ should be one-fifth of $P_\infty(T < 1000)$, i.e., 0.01. We see that only T_3 achieves this rate. Both T_1 and T_2 have significantly higher early stop rates. This is because $Z_{|y}(t, n)$ becomes more left skewed when t/n becomes smaller. This means that, for the same amount of change Δ , T_1 and T_2 could detect the change much easier if it occurs earlier, while much harder if it occurs later. In reality, the change may occur at very large n , then the signal needs to be really large for T_1 or T_2 to detect. This could be a big issue for anomaly detection.

By considering all these, we recommend to use T_3 in practice. Even though T_3 is less powerful than T_1 and T_2 according to the failure II rate, this can usually be easily fixed by including slightly more NNs into the test. On the other hand, T_3 has the desirable property of uniform false discovery rate along time. In other words, no matter when the change happens, its power of detection is the same. Furthermore, the computation time for T_3 is much less than T_1 and T_2 when n is large, which is also preferred in real applications.

In the following, we focus on the stopping rule T_3 . If not further noted, T and b refer to T_3 and b_3 , respectively, in the rest of the paper.

4. Average run length $E_\infty(T(b))$. Given the stopping rule $T(b)$, the remaining question is how to determine the detection threshold b , in particular, how to choose b so that the average run length $E_\infty(T(b))$ is a pre-specified value, such as 10,000.

First of all, we usually don’t know the underlying distribution of the observations, so we couldn’t directly simulate observations to obtain b as done in Section 3.1. Secondly, resampling based methods, such as permutation and bootstrap, are not appropriate here as new observations keep arriving and the limited existing observations are usually not representative enough, especially for complicated data. Even if one could come up with some approaches through resampling methods, they would be very time consuming and not practical for online applications. Therefore, we seek to obtain an analytic formula for $E_\infty(T(b))$.

Given the non-parametric nature of the proposed method, we would not be able to get an exact analytic formula for $E_\infty(T(b))$ for finite L , the number of observations used at each time, so we approach the problem asymptotically, i.e., $L \rightarrow \infty$. We then make further modifications so that the analytic formula is a good

approximation for finite L .

4.1. Asymptotic results. We first consider the asymptotic scenario, $L \rightarrow \infty$. In this context, $\{Z_{L|\mathbf{y}}(t, n)\}_{t, n}$, with t and n rescaled by L , can be shown to converge to a two-dimensional Gaussian random field under very mild conditions. The properties of the supremum of a two-dimensional Gaussian random field was well studied ([Siegmund and Venkatraman, 1995](#)), and the remaining task is to quantify the covariance function of the Gaussian random field, as well as its partial derivatives. They can be obtained by studying the dynamics of the NN relations. The main results are given in Lemma [4.1](#) and Theorems [4.2](#) and [4.4](#).

We assume the following condition.

CONDITION 1. *There is a positive constant \mathbb{C} , $1 \leq \mathbb{C} < \infty$, depending only on k , such that*

$$\sup_{1 \leq j \leq n} \left(\sum_{i=1}^n A_{n,ij}^+ \right) \leq \mathbb{C}, \quad n \in \mathbb{N}.$$

In k -NN, each observation points to its first k NNs, so the out-degree of each observation (the number of arrows pointing from the observation) is k , while the in-degree of each observation (the number of arrows pointing to the observation) can vary. This condition says that the in-degree of each observation is bounded. It is satisfied almost surely for multivariate data ([Bickel and Breiman, 1983](#); [Henze, 1988](#)). For non-Euclidean data, if the distance is chosen properly, this condition is also easy to hold as many non-Euclidean data can be embedded into a Euclidean space.

Before stating the main results, we define some useful quantities. According to Propositions 3.1 and 3.2 in [Henze \(1988\)](#), under Condition 1, the quantities

$$\frac{1}{L} \sum_{i,j \in n_L} A_{n_L,ij}^{(r)} A_{n_L,ji}^{(s)}, \quad \frac{1}{L} \sum_{i,j,l \in n_L, j \neq l} A_{n_L,ji}^{(r)} A_{n_L,li}^{(s)},$$

converge in probability to constants as $L \rightarrow \infty$ and the limits can be calculated through complicated integrals ([Henze, 1988](#)). We denote the limits as

$$p_\infty(r, s) = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{i,j \in n_L} A_{n_L,ij}^{(r)} A_{n_L,ji}^{(s)}, \quad (4.1)$$

$$q_\infty(r, s) = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{i,j,l \in n_L, j \neq l} A_{n_L,ji}^{(r)} A_{n_L,li}^{(s)}. \quad (4.2)$$

Let

$$p_{k,\infty} = \sum_{r=1}^k \sum_{s=1}^k p_\infty(r, s), \quad (4.3)$$

$$q_{k,\infty} = \sum_{r=1}^k \sum_{s=1}^k q_\infty(r, s). \quad (4.4)$$

Then $p_{k,\infty}$ is the limiting expected number of mutual NNs a node has in k -NN and $q_{k,\infty}$ the limiting expected number of nodes that share a NN with a node in k -NN. We also define their finite sample versions by taking expectations:

$$p_L(r, s) = \frac{1}{L} \mathbb{E} \left(\sum_{i,j \in n_L} A_{n_L,ij}^{(r)} A_{n_L,ji}^{(s)} \right), \quad (4.5)$$

$$q_L(r, s) = \frac{1}{L} \mathbb{E} \left(\sum_{i,j,l \in n_L, j \neq l} A_{n_L,ji}^{(r)} A_{n_L,li}^{(s)} \right), \quad (4.6)$$

$$p_{k,L} = \frac{1}{L} \mathbb{E} \left(\sum_{i,j \in n_L} A_{n_L,ij}^+ A_{n_L,ji}^+ \right), \quad (4.7)$$

$$q_{k,L} = \frac{1}{L} \mathbb{E} \left(\sum_{i,j,l \in n_L, j \neq l} A_{n_L,ji}^+ A_{n_L,li}^+ \right). \quad (4.8)$$

Then

$$\begin{aligned} \lim_{L \rightarrow \infty} p_L(r, s) &= p_\infty(r, s), \quad \lim_{L \rightarrow \infty} q_L(r, s) = q_\infty(r, s), \\ \lim_{L \rightarrow \infty} p_{k,L} &= p_{k,\infty}, \quad \lim_{L \rightarrow \infty} q_{k,L} = q_{k,\infty}. \end{aligned}$$

We next state the main results.

LEMMA 4.1. *Under Condition 1, when $t - (n - L)$, $(n - t) = O(L)$, as $L \rightarrow \infty$, $Z_{L|\mathbf{y}}(t, n) \rightarrow Z_L(t, n)$ almost surely, where*

$$Z_L(t, n) = -\frac{R_L(t, n) - \mathbb{E}(R_L(t, n))}{\sqrt{\text{Var}(R_L(t, n))}}.$$

This lemma follows immediately from Propositions 3.1 and 3.2 in Henze (1988).

THEOREM 4.2. *Under Condition 1, as $L \rightarrow \infty$, the finite dimensional distributions of $\{Z_L([vL], [wL]) : 0 < w - 1 < v < w < \infty\}$ weakly converges to the finite dimensional distributions of a two-dimensional Gaussian random field, which we denote as $\{Z^*(v, w) : 0 < w - 1 < v < w < \infty\}$. (Here, $[x]$ denotes the largest integer smaller than or equal to x for any real number x .)*

A main challenge to prove this theorem is how to deal with the holistic dependencies among $A_{n_L,ij}^+$'s. Even for different i, j, l, r , $A_{n_L,ij}^+$ and $A_{n_L,lr}^+$ are dependent. This is because of the constraints $\sum_j A_{n_L,ij}^+ = k$ for all $i \in n_L$ (see details in Appendix A.1).

We consider a similar set of Bernoulli random variables $\{\tilde{A}_{n_L,ij}^+\}_{i,j \in n_L}$ but with relaxed dependencies. We keep the following probabilities unchanged:

$$\mathbb{P}(\tilde{A}_{n_L,ij}^+ = 1) = \mathbb{P}(A_{n_L,ij}^+ = 1),$$

$$\begin{aligned} \mathbb{P}(\tilde{A}_{n_L,ij}^+ = 1, \tilde{A}_{n_L,ji}^+ = 1) &= \mathbb{P}(A_{n_L,ij}^+ = 1, A_{n_L,ji}^+ = 1), \\ \mathbb{P}(\tilde{A}_{n_L,ji}^+ = 1, \tilde{A}_{n_L,li}^+ = 1) &= \mathbb{P}(A_{n_L,ji}^+ = 1, A_{n_L,li}^+ = 1). \end{aligned}$$

That is, two-way NN relations are retained. However, we relax the other dependencies. We let $\tilde{A}_{n_L,ij}^+$ be independent of $\{\tilde{A}_{n_L,il}^+, \tilde{A}_{n_L,li}^+\}_{l \neq j}$. We also let $\tilde{A}_{n_L,ij}^+$ and $\tilde{A}_{n_L,lr}^+$ be independent when i, j, l, r are all different.

Then $\tilde{A}_{n_L,ij}^+$'s are only locally dependent. But $\sum_j \tilde{A}_{n_L,ij}^+$'s are no longer necessarily k . However, $\{\tilde{A}_{n_L,ij}^+\}_{i,j \in n_L}$ becomes $\{A_{n_L,ij}^+\}_{i,j \in n_L}$ if we condition on the events $\left\{\sum_j \tilde{A}_{n_L,ij}^+ = k\right\}_{i \in n_L}$. Thus, $Z_L(t, n)$ can be studied through the joint distribution of summations of locally dependent terms. We then use Stein's method to deal with local dependencies. The complete proof is in Appendix A.1.

REMARK 4.3. *The tightness of the two-dimensional field shall be able to be shown for $\{Z_L([vL], [wL]) : 0 < w - 1 + \delta \leq v \leq w - \delta < \infty\}$ for any $\delta \in (0, 1)$. For v too close to $w - 1$ or w , the fluctuation in the random field could be too wild to have the field being uniformly tight.*

Based on Theorem 4.2, we approximate $\mathbb{E}_\infty(T(b))$ by that of the corresponding quantity defined for the limiting random field:

$$T^*(b) = \inf \left\{ n - N_0 : \left(\max_{n-n_1 \leq t \leq n-n_0} Z^*(t/L, n/L) \right) > b, n \geq N_0 \right\}. \quad (4.9)$$

According to Siegmund and Venkatraman (1995), when $b, L, n_0, n_1 \rightarrow \infty$ in such a way that $b = c\sqrt{L}$ for some fixed $0 < c < \infty$, $n_0 = u_0 L$ and $n_1 = u_1 L$ for some fixed $0 < u_0 < u_1 < 1$, and when there is no change point, $T^*(b)$ is asymptotically exponentially distributed with mean

$$\mathbb{E}_\infty(T^*(b)) \sim \frac{\sqrt{2\pi} \exp(b^2/2)}{c^2 b \int_{u_0}^{u_1} g_1(u) g_2(u) \nu \left(c\sqrt{2g_1(u)} \right) \nu \left(c\sqrt{2g_2(u)} \right) du}, \quad (4.10)$$

where

$$\begin{aligned} g_1(u) &= \left. \frac{\partial_- \rho_{(u,w)}^*(\delta_1, 0)}{\partial \delta_1} \right|_{\delta_1=0} \equiv - \left. \frac{\partial_+ \rho_{(u,w)}^*(\delta_1, 0)}{\partial \delta_1} \right|_{\delta_1=0}, \\ g_2(u) &= \left. \frac{\partial_- \rho_{(u,w)}^*(0, \delta_2)}{\partial \delta_2} \right|_{\delta_2=0} \equiv - \left. \frac{\partial_+ \rho_{(u,w)}^*(0, \delta_2)}{\partial \delta_2} \right|_{\delta_2=0}, \\ \nu(x) &= 2x^{-2} \exp \left\{ -2 \sum_{m=1}^{\infty} m^{-1} \Phi \left(-\frac{1}{2} x m^{1/2} \right) \right\}, \quad x > 0. \end{aligned}$$

Here, $\rho_{(u,w)}^*(\delta_1, \delta_2) = \text{Cov}(Z^*(w-u, w), Z^*(w-u+\delta_1, w+\delta_2))$ and $\nu(\cdot)$ is closely related to the Laplace transform of the overshoot over the boundary of a random

walk. A simple approximation given in [Siegmund and Yakir \(2007\)](#) is sufficient for numerical purpose:

$$\nu(x) \approx \frac{(2/x)(\Phi(x/2) - 0.5)}{(x/2)\Phi(x/2) + \phi(x/2)}, \quad (4.11)$$

where $\Phi(\cdot)$ is the cumulate distribution function of the standard normal distribution and $\phi(\cdot)$ the density function of the standard normal distribution.

Thus, the remaining task is to derive the directional partial derivatives of the covariance function of the Gaussian random field. Their analytic expressions are given in the following theorem.

THEOREM 4.4. *For the two-dimensional field $\{Z^*(v, w) : 0 < w - 1 < v < w < \infty\}$, the directional partial derivatives are*

$$\begin{aligned} g_1(u) &= \left. \frac{\partial_- \rho_{(u,w)}^*(\delta_1, 0)}{\partial \delta_1} \right|_{\delta_1=0} \equiv - \left. \frac{\partial_+ \rho_{(u,w)}^*(\delta_1, 0)}{\partial \delta_1} \right|_{\delta_1=0} \\ &= \frac{16u(1-u)(k + p_{k,\infty}) + 2(1-2u)^2(q_{k,\infty} - k^2 + k)}{\sigma^2(u)}, \end{aligned} \quad (4.12)$$

$$\begin{aligned} g_2(u) &= \left. \frac{\partial_- \rho_{(u,w)}^*(0, \delta_2)}{\partial \delta_2} \right|_{\delta_2=0} \equiv - \left. \frac{\partial_+ \rho_{(u,w)}^*(0, \delta_2)}{\partial \delta_2} \right|_{\delta_2=0} \\ &= \frac{16u^2(1-u)^2(p_{k,\infty} + q_{k,\infty} + k^2 + 2p_{k,\infty}^{(k)} - 2q_{k,\infty}^{(k)})}{\sigma^2(u)} \\ &\quad + \frac{4u(1-u)(2q_{k,\infty}^{(k)} - 3q_{k,\infty} + k^2 + k) + 2(q_{k,\infty} - k^2 + k)}{\sigma^2(u)}, \end{aligned} \quad (4.13)$$

where

$$\begin{aligned} \sigma^2(u) &= 4u(1-u)(4u(1-u)(k + p_{k,\infty}) + (1-2u)^2(q_{k,\infty} - k^2 + k)), \\ p_{k,\infty}^{(k)} &= \sum_{r=1}^k p_\infty(k, r), \quad q_{k,\infty}^{(k)} = \sum_{r=1}^k q_\infty(k, r). \end{aligned}$$

The complete proof of this theorem is in [Appendix A.2](#). We studied the dynamics of the k -NN series as new observations are added through combinatorial analysis and it turned out that a few key quantities are enough to characterize the dynamics in the asymptotic domain.

4.2. Finite L . We now consider the practical scenario where L is finite. Based on [Theorems 4.2 and 4.4](#), $E_\infty(T(b))$ can be approximated by

$$E_\infty(T(b)) \approx \frac{L\sqrt{2\pi}\exp(b^2/2)}{b^3 \int_{\frac{n_0}{L}}^{\frac{n_1}{L}} g_1(u)g_2(u)\nu\left(\sqrt{2b^2g_1(u)/L}\right)\nu\left(\sqrt{2b^2g_2(u)/L}\right)du}$$

with the analytic expressions for $g_1(u)$ and $g_2(u)$ given in (4.12) and (4.13), respectively, and $\nu(\cdot)$ given in (4.11).

When deriving the limiting expressions for $g_1(u)$ and $g_2(u)$, we evaluate $\sum_j \mathbb{E} \left(A_{n_L,ij}^{(r)} A_{n_L,ji}^{(s)} \right)$ and $\sum_{j \neq l} \mathbb{E} \left(A_{n_L,ji}^{(r)} A_{n_L,li}^{(s)} \right)$ under $L \rightarrow \infty$ and the two quantities become $p_\infty(r, s)$ and $q_\infty(r, s)$, respectively. In practice, when L is finite, $p_\infty(r, s)$ and $q_\infty(r, s)$ are not the best estimates for these two expectations, yet the expectations could be better estimated through historical data. Therefore, we use the following formula to approximate $\mathbb{E}_\infty(T(b))$ in practice:

$$\mathbb{E}_\infty(T(b)) \approx \frac{L\sqrt{2\pi} \exp(b^2/2)}{b^3 \int_{\frac{n_0}{L}}^{\frac{n_1}{L}} g_{L,1}(u) g_{L,2}(u) \nu \left(\sqrt{2b^2 g_{L,1}(u)/L} \right) \nu \left(\sqrt{2b^2 g_{L,2}(u)/L} \right) du} \quad (4.14)$$

where $g_{L,1}(u)$ and $g_{L,2}(u)$ are the same as $g_1(u)$ and $g_2(u)$, respectively, except that $p_{k,\infty}$, $q_{k,\infty}$, $p_{k,\infty}^{(k)}$ and $q_{k,\infty}^{(k)}$ are replaced by $p_{k,L}$, $q_{k,L}$, $p_{k,L}^{(k)}$ and $q_{k,L}^{(k)}$, respectively, with $p_{k,L}$ given in (4.7), $q_{k,L}$ given in (4.8), and

$$p_{k,L}^{(k)} = \sum_{r=1}^k p_L(k, r), \quad q_{k,L}^{(k)} = \sum_{r=1}^k q_L(k, r). \quad (4.15)$$

For $p_{k,L}$, $q_{k,L}$, $p_{k,L}^{(k)}$ and $q_{k,L}^{(k)}$, they usually don't have analytical expressions. However, they can be easily estimated from historical data. These estimates can further be updated by new observations as long as no change point is detected.

We next check how this analytic approximation works. We compare the threshold b such that $\mathbb{E}_\infty(T(b)) = 10,000$ based on this analytic approximation and that based on 10,000 Monte Carlo simulations. The threshold obtained through 10,000 Monte Carlo simulations can be regarded as the true threshold. Results under different choices of n_0 , k and d for multivariate Gaussian data are shown in Table 2. We checked two values of L , namely $L = 200$ and $L = 50$, and let $n_1 = L - n_0$.

Unfortunately, the thresholds obtained through the analytic approximation (4.14) are not that close to the Monte Carlo results except for a few occasions. The analytic approximation (4.14) gives similar thresholds for different dimensions when all other parameters are fixed. However, the thresholds from Monte Carlo simulations are quite different for different dimensions with those under a higher dimension much smaller. Thus, (4.14) is still missing some major components for finite L due to the fact that $Z_L(t, n)$ can be quite left skewed for finite L and small $(n - t)$. In the following, we incorporate skewness of $Z_L(t, n)$ to improve the analytic approximation.

4.2.1. Skewness correction. We adapt the skewness correction approach in [Chen and Zhang \(2015\)](#). In particular, when we derive the average run length for the limiting two-dimensional Gaussian random field (4.10), the term in the integral related to the marginal distribution of $Z^*(w - u, w)$ is $\mathbb{P}(Z^*(w - u, w) \in b + du)$. (Here, du is the differential of the variable u , and similar definition for dt in the

TABLE 2

The threshold b , such that $E_\infty(T(b)) = 10,000$, through 10,000 Monte Carlo simulations, through analytic formula (4.14) based on asymptotic results, and through analytic formula (4.17) with additional skewness correction. Each observation in the data sequence follows a d -dimensional normal distribution.

		$n_0 = 3$			$n_0 = 10$		
		Monte Carlo	Asymp. (4.14)	Skewness Corrected (4.17)	Monte Carlo	Asymp. (4.14)	Skewness Corrected (4.17)
L = 200							
$d = 10$	$k = 1$	4.04	4.40	4.07	4.04	4.31	4.07
	$k = 3$	4.14	4.34	4.14	4.14	4.23	4.14
	$k = 5$	4.16	4.31	4.18	4.16	4.17	4.18
$d = 100$	$k = 1$	3.76	4.37	3.79	3.76	4.26	3.79
	$k = 3$	3.78	4.33	3.79	3.78	4.20	3.79
	$k = 5$	3.79	4.31	3.81	3.79	4.18	3.81
$d = 1000$	$k = 1$	3.73	4.38	3.73	3.73	4.28	3.73
	$k = 3$	3.71	4.33	3.71	3.71	4.21	3.71
	$k = 5$	3.75	4.32	3.72	3.75	4.18	3.72
$d = 10000$	$k = 1$	3.71	4.38	3.70	3.71	4.27	3.70
	$k = 3$	3.65	4.33	3.69	3.65	4.21	3.69
	$k = 5$	3.68	4.32	3.69	3.68	4.18	3.69
L = 50							
$d = 10$	$k = 1$	4.00	4.38	4.10	3.99	4.24	4.10
	$k = 3$	4.36	4.32	4.37	4.36	4.19	4.37
	$k = 5$	4.57	4.28	4.50	4.57	4.15	4.50
$d = 100$	$k = 1$	3.86	4.36	3.94	3.83	4.23	3.94
	$k = 3$	3.92	4.31	4.02	3.92	4.18	4.02
	$k = 5$	3.95	4.29	4.09	3.95	4.15	4.09
$d = 1000$	$k = 1$	3.83	4.36	3.91	3.83	4.23	3.91
	$k = 3$	3.92	4.32	3.93	3.92	4.18	3.93
	$k = 5$	3.95	4.29	3.97	3.95	4.15	3.97
$d = 10000$	$k = 1$	3.79	4.36	3.90	3.79	4.23	3.90
	$k = 3$	3.86	4.32	3.90	3.86	4.18	3.90
	$k = 5$	3.91	4.29	3.92	3.91	4.15	3.92

following.) To make the analytic approximation more accurate for finite L and small n_0 , we replace $\mathbf{P}(Z^*(w-u, w) = b+du)$ by an estimate of $\mathbf{P}(Z_L([n(w-u)], [nw]) \in b+du)$. Following the method based on cumulant-generating functions and change of measure (details refer to [Chen and Zhang \(2015\)](#)), we have

$$\begin{aligned} & \frac{\mathbf{P}(Z_L(t, n) \in b+dt/b)}{\mathbf{P}(Z^*(n/L-t/L, n/L) \in b+dt/b)} \\ & \approx \frac{\exp((b-\theta_b)^2/2 + \theta_b^2 \gamma_L(t, n) \theta_b/6)}{\sqrt{(1+\gamma_L(t, n) \theta_b)}} := S_L((n-t)/L). \end{aligned} \quad (4.16)$$

Here, $\theta_b = (-1 + \sqrt{1 + 2\gamma_L(t, n)b})/\gamma_L(t, n)$ and $\gamma_L(t, n) = \mathbf{E}(Z_L^3(t, n))$. The denotation for $S_L((n-t)/L)$ holds because $\gamma_L(t, n)$ relates to t and n only as a function of $n-t$ (see Lemma 4.5 below). Then, the analytic approximation for $\mathbf{E}_\infty(T)$ incorporating skewness becomes

$$\frac{L\sqrt{2\pi} \exp(b^2/2)}{b^3 \int_{n_0/L}^{n_1/L} \mathbf{S}_L(\mathbf{u}) g_{L,1}(u) g_{L,2}(u) \nu\left(\sqrt{2b^2} g_{L,1}(u)/L\right) \nu\left(\sqrt{2b^2} g_{L,2}(u)/L\right) du}. \quad (4.17)$$

When $L \rightarrow \infty$ and $(n-t), (L-(n-t)) = O(L)$, $\gamma_L(t, n)$ goes to 0 and $S_L(u)$ goes to 1 for $0 < u < 1$, so this formula converges to (4.10) in the limit.

The exact analytic expression for $\gamma_L(t, n)$ is given in the following lemma:

LEMMA 4.5. *We have*

$$\gamma_L(t, n) = \frac{(E(R_L(t, n)))^3 + 3E(R_L(t, n))\text{Var}(R_L(t, n)) - E(R_L^3(t, n))}{(\text{Var}(R_L(t, n)))^{3/2}},$$

where $E(R_L(t, n))$ and $\text{Var}(R_L(t, n))$ are given in (A.3) and (A.4), respectively, and

$$\begin{aligned} E(R_L^3(t, n)) &= 8k^3 L^3 r_4 + 12k^2 L^2 (r_2 + 3k(r_2 - 2r_4)) \\ &+ 4kL(3r_2 - r_1 + 2r_3 - 4r_4 + 3k(3r_1 - 2r_2 - 4r_3 - 4r_4) + 8k^2(r_3 - 3r_2 + 5r_4)) \\ &+ 24p_{k,L}(kL^2 r_4 + kL(r_1 + r_2 - 2r_3 - 4r_4) + 2L(2r_3 - r_1 + 2r_4)) \\ &+ 12q_{k,L}(kL^2(r_2 - 2r_4) + kL(2r_3 - 5r_2 + 8r_4) + L(r_1 + r_2 - 2r_3 - 4r_4)) \\ &+ 4(2r_3 - 3r_2 + 4r_4) E\left(\sum_{i,j,l,v} A_{n_L,ji}^+ A_{n_L,li}^+ A_{n_L,vi}^+\right) \\ &+ 24(r_1 + r_2 - 2r_3 - 4r_4) E\left(\sum_{i,j,l} A_{n_L,ij}^+ A_{n_L,ji}^+ A_{n_L,li}^+\right) \\ &+ 24(2r_4 - r_2) E\left(\sum_{i,j,l,v} A_{n_L,ij}^+ A_{n_L,li}^+ A_{n_L,vj}^+\right) \\ &- 16r_4 \left(E\left(\sum_{i,j,l} A_{n_L,ij}^+ A_{n_L,jl}^+ A_{n_L,li}^+\right) + 3E\left(\sum_{i,j,l} A_{n_L,ij}^+ A_{n_L,il}^+ A_{n_L,jl}^+\right) \right) \end{aligned}$$

with

$$\begin{aligned}
 r_1 &= \frac{2x(L-x)}{L(L-1)}, \quad x = L - (n-t), \\
 r_2 &= \frac{4x(x-1)(L-x)(L-x-1)}{L(L-1)(L-2)(L-3)}, \\
 r_3 &= \frac{x(L-x)((x-1)(x-2) + (L-x-1)(L-x-2))}{L(L-1)(L-2)(L-3)}, \\
 r_4 &= \frac{8x(x-1)(x-2)(L-x)(L-x-1)(L-x-2)}{L(L-1)(L-2)(L-3)(L-4)(L-5)}.
 \end{aligned}$$

To prove this lemma, we have

$$\begin{aligned}
 \mathbb{E}(R_L^3(t, n)) &= \mathbb{E}(\mathbb{E}(R_L^3(t, n) | \mathbf{Y})) \\
 &= \sum_{i,j,l,r,u,v} \mathbb{E} \left((A_{n_L,ij}^+ + A_{n_L,ji}^+)(A_{n_L,lr}^+ + A_{n_L,rl}^+)(A_{n_L,uv}^+ + A_{n_L,vu}^+) \right) \\
 &\quad \times \mathbb{E}(B_{ij}(t, n_L)B_{lr}(t, n_L)B_{lr}(t, n_L)).
 \end{aligned}$$

Adapting similar arguments in calculating the covariance in the proof of Theorem 4.4 but with more careful treatment of the summation indices, we could get the result in the lemma.

From Lemma 4.5, we see that $\mathbb{E}(R_L^3(t, n))$ depends on the probability of having certain structures in the nearest neighbor graph. The relevant structures in k -NN are shown in Figure 2. The first two structures represent mutual NNs and shared NNs. The other five structures are three-way interactions among the NN relations. The probability of having each of them can be estimated through historical data, and can also be updated by new observations when no change point is detected.



FIG 2. The configurations in k -NN that relate to the third moment of $R_L(t, n)$.

We now check how skewness correction performs. Table 2 also lists the thresholds obtained through the analytic approximation with skewness correction. We see that, after skewness correction, the analytic formula gives much better estimates to the thresholds. When $L = 200$, all thresholds estimated by (4.17) are very accurate. Even for small L ($L = 50$), the analytic approximated with skewness correction is doing a reasonable job. When the dimension becomes larger, the threshold estimated by the analytic formula with skewness correction is smaller, exhibiting the same trend as the Monte Carlo results.

These results show that the formula with skewness correction could capture the major factors and gives quite reliable estimates. It would be reasonable to use the analytic formula with skewness correction to get the threshold b in real applications.

5. Power analysis. Given the procedure and the fast analytic way of determining the detection threshold, the proposed method can be easily applied to real problems. Now, the question is how powerful this method is. To get some idea, we compare it to the test based on Hotelling’s T^2 test for multivariate Gaussian data as Hotelling T^2 test is asymptotically the most powerful for testing two multivariate Gaussian distributions with the same covariance matrix.

The simulation setup is as follows: There are $N_0 = 200$ historical observations and a change occurs at $t = 400$ (200 new observations after the start of the test). The observations are independent and follow d -dimensional Gaussian distribution with a mean shift (Δ) at the change-point. (The L_2 distance between the two means is Δ .) The amount of change, Δ , is chosen so that the tests have moderate power. Results are given in Table 3. “Successful detection” is defined the same as in Section 3.1 that the test detects the change point within 100 observations after the change occurred. We compare all tests on the same ground by controlling the early stop probability to be 0.01.

TABLE 3
Fraction of trials (out of 1,000) that the change point is successfully detected for the proposed test and for the test based on the Hotelling’s T^2 test.

	Normal data				Log-normal data	
	$d = 10$ $\Delta = 0.7$	$d = 100$ $\Delta = 1.8$	$d = 1000$ $\Delta = 2.7$	$d = 10000$ $\Delta = 5$	$d = 10$ $\Delta = 1.5$	$d = 100$ $\Delta = 2$
Proposed test: 1-NN	0.02	0.21	0.12	0.16	0.48	0.08
Proposed test: 3-NN	0.07	0.55	0.41	0.52	0.87	0.48
Proposed test: 5-NN	0.15	0.81	0.57	0.70	0.95	0.77
Hotelling’s T^2	0.69	0.63	—	—	0.34	0.02

Table 3 shows the results under different scenarios with 1,000 simulation runs for each scenario. The fraction of the runs that the change point is successfully detected is reported. When the data is multivariate Gaussian, we see that the test based on the Hotelling T^2 test is doing very well in low dimension. When the dimension becomes higher, the power of the proposed test catches up. When $d = 100$, the proposed test based on 5-NN is outperforming the test based on the Hotelling T^2 test. When d is even higher, the dimension is larger than the number of observations that the method based on the Hotelling’s T^2 cannot be applied. For the proposed tests, we see that the we do need to increase the strength of the signal to achieve a similar detection power. However, the number of fold we need for the increase of the signal is much smaller than that for the dimension. When the dimension increase from 100 to 10000 (by a fold of 100), we only need to increase the signal by a fold about 3 to achieve the same detection power. Hence, the proposed method is relatively mildly affected by the dimensionality.

We also did the comparison for log-normal data and the change is in the mean parameter. Now, the assumptions for the Hotelling T^2 test do not hold and we see that the proposed test is outperforming the test based on the Hotelling T^2 test even when the dimension is low.

The results show that the proposed test has satisfying power and works for

various distributions.

6. Real data applications. Here, we apply the proposed method to two real datasets, one on text analysis and the other on network analysis. Both datasets are completely observed at the time of analysis. We treat them as if the data were being observed to illustrate how the proposed method works. In real time, similar analysis as the text analysis example might be applied to detect epidemic disease outbreaks when online search results are used. The search inquiries on related topics could be represented as a count vector. For the network data example, it is conceivable to apply the proposed method in a sequential manner if the data keep arriving.

6.1. Authorship debate. *Tirant lo Blanch* is a chivalry novel published in 1490. It was written in Catalan and played a significant role in the western literature. It is well recognized to have a major influence on the well-known novel *Don Quixote*.

However, there is a long lasting debate on the authorship of the novel. In its first published version, the dedicatory letter at the beginning of the book says that the book was all written by knight *Joanot Martorell*. However, the colophon at the end of the book says that Joanot Martorell died before he finished this book and the last quarter of the book was written by another knight *Marti Joan de Galba*. Since Joanot Martorell was already dead when the book was published, no one knows the truth. People have been debating on this issue for centuries and there is still no consensus ([Girón, Ginebra and Riba, 2005](#)).

Of course, we would not be able to find out the ground truth. However, we can approach this problem objectively by testing if there is any change in writing style because different people have different writing styles. This book has 487 chapters and we test whether there is a change of writing style along the chapters.

We use the word length data provided by J. Girón to represent the writing style. Word length information is well accepted in linguistic studies for characterizing writing styles. In each chapter, the words are categorized by their lengths. Category 1 contains all words with 1 character, category 2 all words with 2 characters, and so on. For words with more than 9 characters, they are put into one category. Figure 3 is a snapshot of the counts on these categories over all chapters. In the following analysis, we use 425 chapters that have more than 200 words.

In this authorship debate, both sides agree that the first three quarters of the book was written by Joanot Martorell. We can use them as the historical observations. In the analysis, we only used the first 100 chapters as the historical observations and test on each of the following chapters to see if any change occurs. To calculate the pairwise distances among the chapters, we first normalize the count vector by dividing its sum. Then the distance of two chapters is defined as the L_2 distance of the normalized vectors.

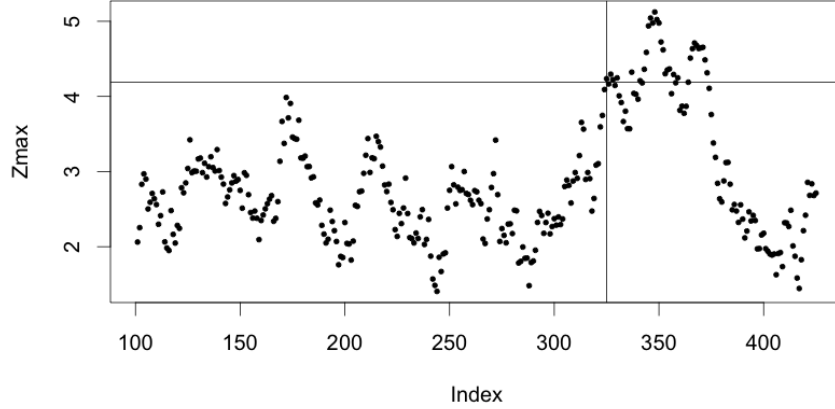
Figure 4 plots $Z_{\max}(n) = \max_{n-L+n_0 \leq t \leq n-n_0} Z_{L|Y}(t, n)$ against n , the chapter index after removing chapters with less than 200 words. We let $L = 100$ and $n_0 = 3$. From (4.17), we have for $E_\infty(T(b)) = 10,000$ the threshold $b = 4.19$.

Since multiple stopping times might be called for one change point, we disregard time n if $\max(Z_{\max}(n-5), Z_{\max}(n-4), \dots, Z_{\max}(n-1)) > b$, i.e., we consider them to be caused by the same event. We call the remaining stopping times the

	1	2	3	4	5	6	7	8	9	10+
Ch1	21	59	44	19	33	20	16	17	9	17
Ch2	53	113	80	49	52	33	28	36	16	16
Ch3	109	274	239	128	112	110	76	51	43	32
Ch4	69	150	126	71	60	71	47	32	23	21
Ch5	119	207	231	123	128	102	61	55	29	34
Ch6	69	136	126	69	60	61	37	27	15	15
...
Ch482	50	47	61	18	32	47	23	32	14	11
Ch483	158	220	207	80	120	93	65	54	62	50
Ch484	59	67	68	37	26	32	15	14	17	6
Ch485	96	174	106	57	77	86	42	54	24	25
Ch486	45	88	91	46	40	28	13	30	11	10
Ch487	48	49	62	53	41	36	21	9	16	13

FIG 3. Word length data (from (Girón, Ginebra and Riba, 2005)).

“candidate stopping times”. We then disregard any candidate stopping time that is within $L/2 - n_0 = 47$ observations from its previous candidate stopping time to avoid double counting on the same change, and call the remaining stopping times the “valid stopping times”

FIG 4. Z_{\max} for the word length data. The horizontal line is the threshold b such that $E_{\infty}(T(b)) = 10,000$. The vertical line is the valid stopping time.

After applying the above rules, we have one valid stopping time at $n = 325$, which corresponds to Chapter 376 in the book, a few chapters after three quarters of the book ($487 \times 0.75 = 365.25$). If there is a change of author, this is likely the place where the change had occurred.

From the results, we see that the writing style of the first three quarters of the book is quite consistent. Moreover, the curve goes below the threshold about 50 chapters after the detected change point and doesn't pass over the threshold

again, indicating that the writing style of the last quarter of the book is also quite consistent, which should be the case as the last quarter of the book was written by the same person according to both sides of the debate. The results support a change of author for this book.

6.2. Friendship network. The MIT Media Laboratory conducted a study following 106 subjects, students and staff in an institute, who used mobile phones with pre-installed software that can record all activities on their phones from July 2004 to June 2005 (Eagle, Pentland and Lazer, 2009). A natural question of interest is whether there is any change in the phone-call pattern among these people over time. This is one way to assess their friendship along time.

We bin the phone calls by day, and for each day, construct a phone-call network with the subjects as nodes and a directed edge pointing from subject i to subject j if subject i called subject j on that day. We encode the directed network of each day by an adjacency matrix, with 1 for element $[i, j]$ if there is a directed edge pointing from subject i to subject j , and 0 otherwise. Let M_i be the 106×106 adjacency matrix on day i . We consider two distance measures defined as:

- (1) the number of different entries: $\|M_i - M_j\|_F^2$, where $\|\cdot\|_F$ means the Frobenius norm of a matrix,
- (2) the number of different entries, normalized by the geometric mean of the total edges in each day: $\frac{\|M_i - M_j\|_F^2}{\|M_i\|_F \|M_j\|_F}$.

For this dataset, since there is no further information to tell whether there is any change point for the first few observations, we applied the offline change-point detection method in Chen and Zhang (2015) on the first 50 days/observations. No change point was found for either distance measure. So we treat the first 50 observations as historical observations. We let $L = 50$, $n_0 = 3$, and determine the threshold based on (4.17).

Figure 5 plots $Z_{\max}(n) = \max_{n-L+n_0 \leq t \leq n-n_0} Z_{L|Y}(t, n)$ against n , the index of days, based on the two distances. The detection thresholds for the two distances are $b = 3.92$ and $b = 3.98$, respectively. Adopting the same rules as in Section 6.1, we find three valid stopping times for distance 1 and six valid stopping times for distance 2. They are summarized in Table 4, together with their nearby academic events.

TABLE 4
Valid stopping times and their nearby academic events.

Distance 1	Distance 2	Nearby academic event*
$n = 66$: 2004/9/23	$n = 60$: 2004/9/17	9/9: First day of class for Fall term
$n = 167$: 2005/1/2	$n = 140$: 2004/12/6	12/18: Last day of class for Fall term
$n = 198$: 2005/2/2	$n = 194$: 2005/1/29	2/2: First day of class for Spring term
—	$n = 229$: 2005/3/5	3/5: Registration deadline for Spring term
—	$n = 252$: 2005/3/28	3/21: Spring vacation
—	$n = 275$: 2005/4/20	4/21: Drop deadline for Spring term

* The dates of the academic events are from the 2015-2016 academic calendar of MIT as the 2004-2005 academic calendar of MIT cannot be found online.

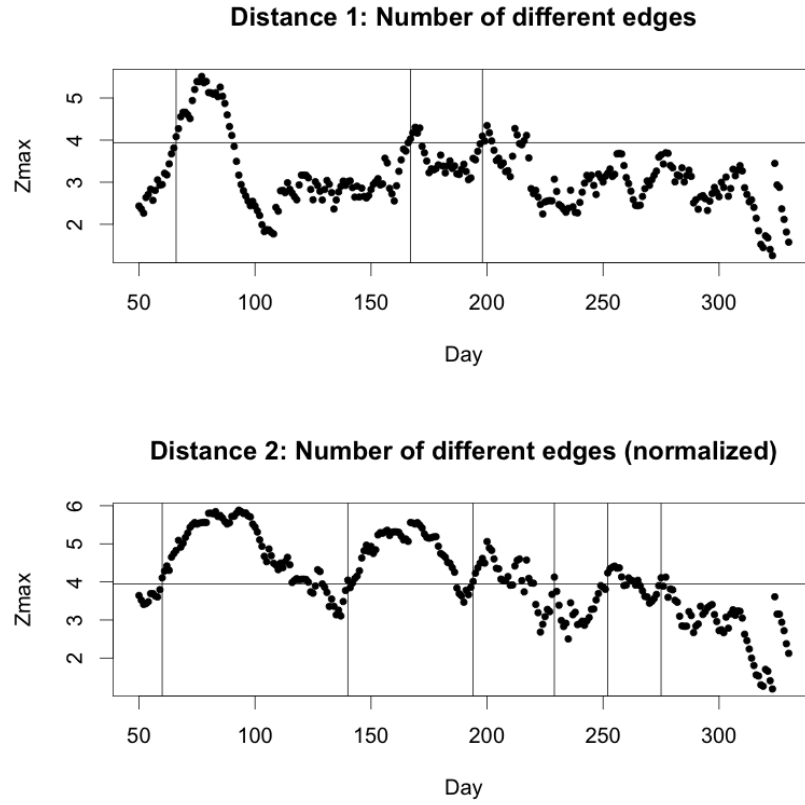


FIG 5. Z_{\max} for the network data based on two distances. The horizontal line in each plot is the threshold b such that $E_{\infty}(T(b)) = 10,000$. The vertical lines are the valid stopping times.

From Table 4, we see that the proposed method based on either distance finds change points at around the beginning of the Fall term, the end of the Fall term, and the beginning of the Spring term. The proposed method using distance 2 finds additional change points in the middle of the Spring term. These are all reasonable times to have some significant call pattern changes.

One may wonder if these change points could be found by a 1-dimensional summary statistic. We plot in Figure 6 the number of edges in each network over time. We could see clearly the change points at around the beginning of the Fall term and the end of the Fall term, reflected by the change of the call volume. Starting from the winter break ($n = 160$), the call volume stabilizes. There is a slight call volume decrease starting from the spring vacation (at around $n = 250$). However, the call volumes from $n = 160$ toward $n = 250$ are quite similar, and there is no significant change within this period. For example, we apply the function `cpt.meanvar()` in R package `changePoint`, a 1-dimensional change-point detection approach for detecting either mean or variance change, to this segment of data and no change point is found. Hence, there is no significant change in the call volume transiting from the winter break to the Spring term.

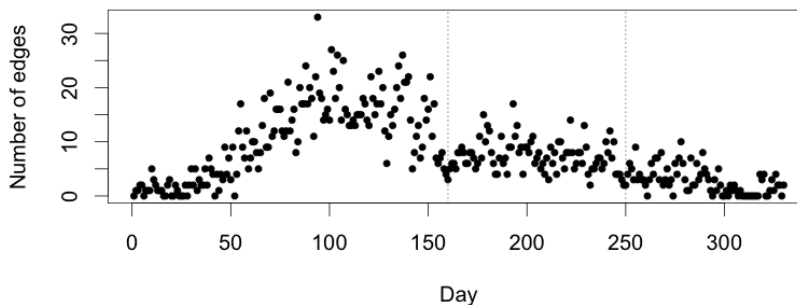


FIG 6. Number of edges in the phone-call network for each day.

On the other hand, the proposed method on either distance finds the change point at the beginning of Spring term (around $n = 198$), indicating that there are some structural changes in the phone-call network which wouldn't be captured by only examining the call volume. Also, since distance 2 is normalized by the total number of edges in each network, there are probably structural changes in the phone-call network besides call volume change in the other five change points detected based on distance 2.

For further details on what the changes are, one could pick some networks before and after the change point and conduct more detailed comparisons. Moreover, if one is interested in some specific characteristics of the network, a distance reflecting such characteristics can be used for the proposed method.

7. Dicussion. In the section, we briefly discuss the choice of k , the number of NNs to be included in the test, and how the test works for gradual changes.

7.1. *Choice of k .* Heuristically, if we choose a very small value of k , some useful similarity information among the observations is not used by the test. We see from Table 3 that the power of the test increases from 1-NN to 5-NN. On the other hand, if we set k to be too large, it may include some irrelevant information, which would also harm the power.

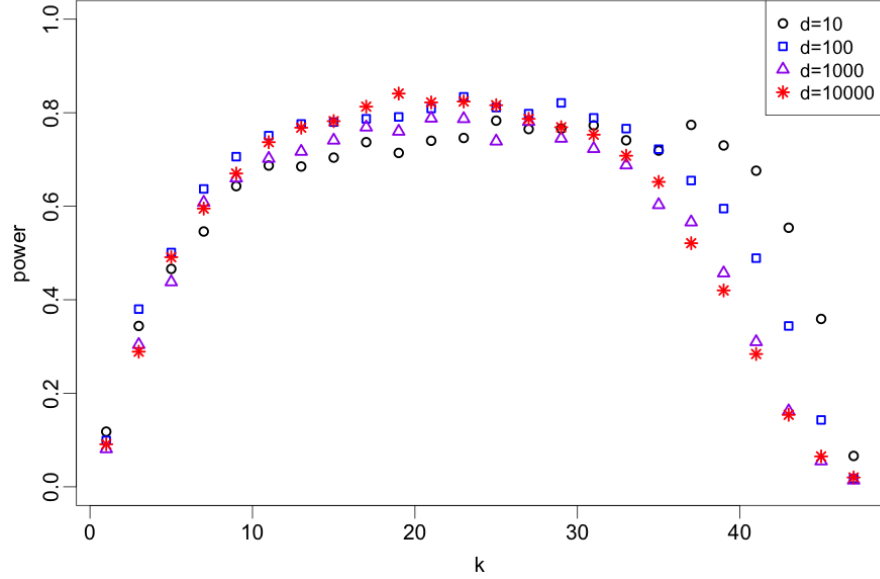


FIG 7. Power of the test based on k -NN for detecting change-points in sequences of multivariate normal data over a range of dimensions: $d = 10$ (black circle), $d = 100$ (blue square), $d = 1000$ (purple triangle), and $d = 10000$ (red star). The change is a shift in mean with the L_2 distance between the means before and after the change Δ : $\Delta = 1.7$ ($d = 10$), $\Delta = 2.7$ ($d = 100$), $\Delta = 4.5$ ($d = 1000$), and $\Delta = 8$ ($d = 10000$). The parameter L is set to be 50, and the power is estimated through 1000 simulation runs.

Figure 7 plots the power of the test as k varies. The different symbols corresponds to different dimensions of the observations. For each dimension, the amount of the change is fixed and only k varies. The amount of the change for each dimension is chosen so that the highest power is around 0.8. We can see clearly from the plot the relation between the power and k : The power first increases as k increases and becomes steady for a wide range of k 's and then decreases as k increases. Therefore, the optimal k should be chosen before the test reaches the plateau to achieve a high power and low computation time at the same time. Another nice thing exhibited by the plot is that the dimension of the observations does not play a significant role in the choice of k . The profiles for different dimensions, from $d = 10$ to $d = 10000$, are almost the same. If we increase the strength of the signal (Figure 8), the whole

curve shifts upward, while the profiles for different dimensions still remain the same.

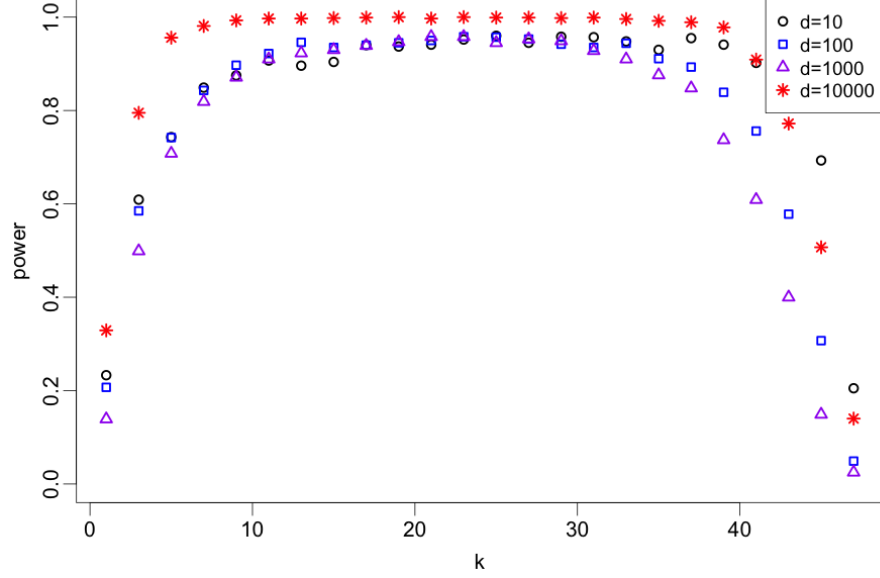


FIG 8. The same set up as in Figure 7 while the strength of the signal is increased for each dimension: $\Delta = 2$ ($d = 10$), $\Delta = 3$ ($d = 100$), $\Delta = 5$ ($d = 1000$), and $\Delta = 10$ ($d = 10000$).

When we set L to be larger (Figure 9, $L = 200$, versus Figure 7, $L = 50$), a similar shape is observed. It is worthwhile to note that the power of the test increases dramatically as L increase: For $d = 1000$, the power achieved by $\Delta = 4.5$ for $L = 50$ is achieved at $\Delta = 2.2$ for $L = 200$. If we set $\Delta = 4$ for $L = 200$, the power is almost 100% for 3-NN and 5-NN (shown as circles in Figure 9).

In practice, for high-dimensional data or non-Euclidean data, sometimes, only large changes may be of interest, then a relative small k would be preferred as large k may detect small changes. On the other hand, if all small changes are of interest, then a relatively large k would be recommended. Also, since the statistics are easy to calculate, it might be helpful to run the detection for a number of k 's simultaneously.

7.2. Gradual change. In some applications, the change may happen gradually rather than abruptly. Even though the proposed method is designed for detecting abrupt changes, it also works for gradual change as long as the change per unit time is relatively strong.

Figure 10 plots the power of the test based on 5-NN for a change of mean. In all scenarios, the L_2 distance between the mean before the change and the mean after the change is 3. However, the change could take more than one unit of time to finish. For example, if the 'gradual change length' is 10, then $\|E(Y_{\tau+9}) - E(Y_{\tau-1})\|_2 = 3$ where τ is the time the change starts to happen. For simplicity,

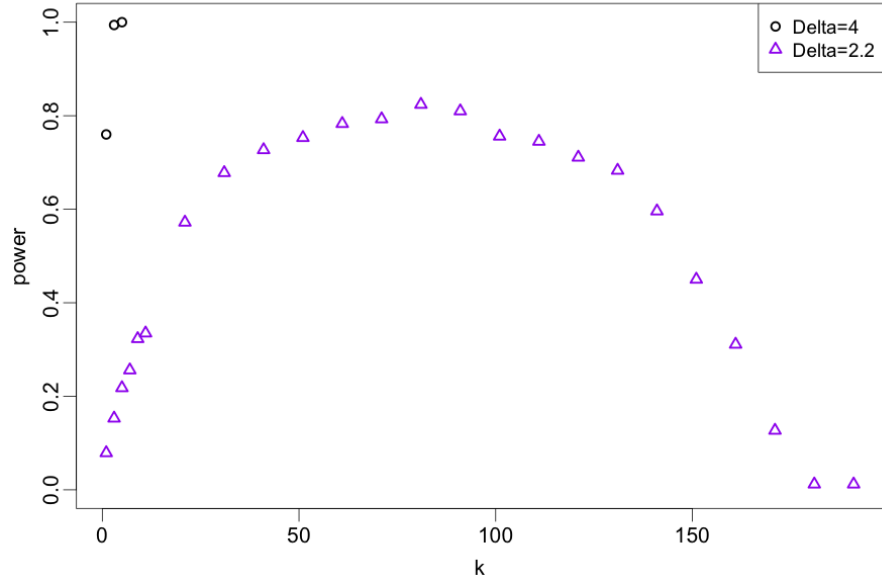


FIG 9. The same set up as in Figure 7 while L is set to be 200. The dimension of the observations in the sequence is 1000.

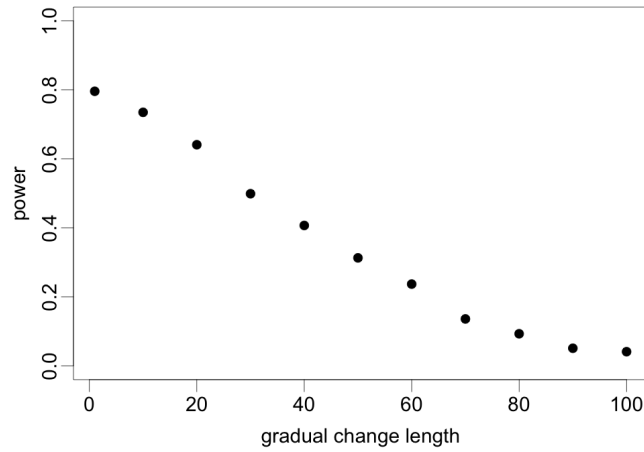


FIG 10. The power of the test based on 5-NN for the same amount of change in the mean with the change speed differs. The 'gradual change length' is the amount of time the change takes to finalize. The longer the gradual change length, the slower the change happens. The dimension of the observations in the sequence is 1000 and L is set to be 200. The power is estimated from 1,000 simulation runs and we call the detection successful if it detects the change within 100 observations from the change starts to happen.

we let the change speed to be the same over the gradual change period. We see that the power decreases as the change takes longer for the same amount of change. However, the decrease in power is not too bad if the length of the change does not take too long to finalize. For example, when the ‘gradual change length’ is 20, the power is 0.64, about 80% of the power if the same amount of change happens abruptly.

8. Conclusion. We propose a new framework for detecting change points sequentially as data are generated. Motivated by the complexity of observations in many real applications, we propose to use nearest neighbor information among the observations for sequential detection. These information can usually be provided by domain experts and thus the proposed method has a wide range of applications.

We explored several stopping rules and the one based on the most recent observations is recommended as it has the desirable property that the detection power is the same across the time. The asymptotic properties of this stopping rule is studied and the analytic approximation for calculating the average run length works well for finite samples after skewness correction. The proposed test exhibits higher power than the parametric method based on normal theory when the dimension of the data is high and/or distributional assumptions for the parametric method are violated. The proposed method is illustrated on the analysis of friendship network data over time and some interesting insights are obtained.

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APPENDIX A: PROOFS FOR LEMMAS AND THEOREMS

A.1. Proof of Theorem 4.2. We here prove that

$$\{Z_L([vL], [wL]) : 0 < w - 1 < v < w < \infty\}$$

converges to a two-dimensional Gaussian random field as $L \rightarrow \infty$. We only need to show that

$$(Z_L([v_1L], [w_1L]), Z_L([v_2L], [w_2L]), \dots, Z_L([v_JL], [w_JL]))$$

converges to a J -dimensional Gaussian distribution as $L \rightarrow \infty$ for any $1 < w_1 < w_2 < \dots < w_J < \infty$, $v_j \in (w_j - 1, w_j)$, $j = 1, \dots, J$ for any fixed J . We show in the following for the case $J = 2$. For $J > 2$, the proof can be done in the same manner but with a more careful treatment of the indices.

To begin the proof, we first take a different perspective of $R_L(t, n)$. Since each permutation can be viewed as another realization of \mathbf{Y} , we can re-write $R_L(t, n)$ as

$$R_L(t, n) = 2 \sum_{i=n-L+1}^t \sum_{j=t+1}^n (A_{nL,ij}^+ + A_{nL,ji}^+).$$

For different $i, j, l \in n_L$, we have

$$\begin{aligned} P(A_{nL,ij}^+ = 1) &= \frac{k}{L-1}, \\ P(A_{nL,ij}^+ = 1, A_{nL,ji}^+ = 1) &= \frac{p_{k,L}}{L-1}, \\ P(A_{nL,ji}^+ = 1, A_{nL,li}^+ = 1) &= \frac{q_{k,L}}{(L-1)(L-2)}. \end{aligned}$$

Since $\sum_{j \in n_L} A_{n_L,ij}^+ = k, \forall i \in n_L$, we have, for different $i, j, l, r \in n_L$,

$$\begin{aligned} P(A_{n_L,ij}^+ = 1, A_{n_L,il}^+ = 1) &= \frac{k(k-1)}{(L-1)(L-2)}, \\ P(A_{n_L,ij}^+ = 1, A_{n_L,li}^+ = 1) &= \frac{k^2 - p_{k,L}}{(L-1)(L-2)}, \\ P(A_{n_L,ij}^+ = 1, A_{n_L,lr}^+ = 1) &= \frac{k^2(L-3) + p_{k,L} - q_{k,L}}{(L-1)(L-2)(L-3)}. \end{aligned}$$

Therefore, $A_{n_L,ij}^+$ and $A_{n_L,lr}^+$ are dependent even when i, j, l, r are all different. Hence, all $A_{n_L,ij}^+$'s ($i, j \in n_L, i \neq j$) are dependent with each other.

We consider a set of $\{\tilde{A}_{n_L,ij}^+\}_{i,j \in n_L}$ that are less dependent than $\{A_{n_L,ij}^+\}_{i,j \in n_L}$. For different $i, j, l \in n_L$, let $\{A_{n_L,ij}^+\}_{i,j \in n_L}$ be Bernoulli random variables with

$$\begin{aligned} P(\tilde{A}_{n_L,ij}^+ = 1) &= \frac{k}{L-1}, \\ P(\tilde{A}_{n_L,ij}^+ = 1, \tilde{A}_{n_L,ji}^+ = 1) &= \frac{pk,L}{L-1}, \\ P(\tilde{A}_{n_L,ji}^+ = 1, \tilde{A}_{n_L,li}^+ = 1) &= \frac{q_{k,L}}{(L-1)(L-2)}. \end{aligned}$$

These quantities are defined the same as those for $A_{n_L,ij}^+$'s. However, we let $\tilde{A}_{n_L,ij}^+$ be independent of $\{\tilde{A}_{n_L,il}^+, \tilde{A}_{n_L,li}^+\}_{l \neq j}$. Also, for different $i, j, l, r \in n_L$, we let $\tilde{A}_{n_L,ij}^+$ and $\tilde{A}_{n_L,lr}^+$ be independent. Then $\{\tilde{A}_{n_L,ij}^+\}_{i,j \in n_L}$ are only locally dependent. However, $\sum_j \tilde{A}_{n_L,ij}^+$'s would no longer be necessarily k . But if we condition on the events $\left\{ \sum_j \tilde{A}_{n_L,ij}^+ = k \right\}_{i \in n_L}$, $\{\tilde{A}_{n_L,ij}^+\}_{i,j \in n_L}$ becomes $\{A_{n_L,ij}^+\}_{i,j \in n_L}$.

We here define

$$\begin{aligned} \tilde{R}_L(t, n) &= 2 \sum_{i=n-L+1}^t \sum_{j=t+1}^n (\tilde{A}_{n_L,ij}^+ + \tilde{A}_{n_L,ji}^+), \\ \tilde{Z}_L(t, n) &= \frac{\tilde{R}_L(t, n) - E(\tilde{R}_L(t, n))}{\sqrt{\text{Var}(\tilde{R}_L(t, n))}}, \\ \tilde{N}_L^{(l)}(t, n) &= \sum_{i=n-L+1}^t \sum_{j \in n_L} \tilde{A}_{n_L,ij}^+, \\ \tilde{N}_L^{(r)}(t, n) &= \sum_{i=t+1}^n \sum_{j \in n_L} \tilde{A}_{n_L,ij}^+, \\ \tilde{M}_L^{(l)}(t, n) &= \frac{\tilde{N}_L^{(l)}(t, n) - E(\tilde{N}_L^{(l)}(t, n))}{\sqrt{\text{Var}(\tilde{N}_L^{(l)}(t, n))}}, \\ \tilde{M}_L^{(r)}(t, n) &= \frac{\tilde{N}_L^{(r)}(t, n) - E(\tilde{N}_L^{(r)}(t, n))}{\sqrt{\text{Var}(\tilde{N}_L^{(r)}(t, n))}}. \end{aligned}$$

Let $x = L - (n - t)$, we have

$$\begin{aligned}
\mathbb{E}(\tilde{R}_L(t, n)) &= \frac{4kx(L-x)}{L-1}, \\
\text{Var}(\tilde{R}_L(t, n)) &= \frac{4x(L-x)}{L-1} \left(2k + 2p_{k,L} + q_{k,L} - \frac{L+2}{L-3}k^2 \right), \\
\mathbb{E}(\tilde{N}_L^{(l)}(t, n)) &= kx, \\
\text{Var}(\tilde{N}_L^{(l)}(t, n)) &= xk - \frac{x^2k^2}{L-1} + \frac{x(x-1)}{L-1}(p_{k,L} + q_{k,L}), \\
\mathbb{E}(\tilde{N}_L^{(r)}(t, n)) &= k(L-x), \\
\text{Var}(\tilde{N}_L^{(r)}(t, n)) &= (L-x)k - \frac{(L-x)^2k^2}{L-1} + \frac{(L-x)(L-x-1)}{L-1}(p_{k,L} + q_{k,L}).
\end{aligned}$$

To show that $Z_L([v_1L], [w_1L])$ and $Z_L([v_2L], [w_2L])$ are jointly normal, we only need to show the following two lemmas. For simplicity, let $t_i = [v_iL]$, $n_i = [w_iL]$, $x_i = L - (n_i - t_i)$, $u_i = w_i - v_i$, $i = 1, 2$. We thus work under the following condition.

CONDITION 2. $(n_1 - t_1), (L - n_1 + t_1), (n_2 - t_2), (L - n_2 + t_2), (n_2 - n_1) = O(L)$.

LEMMA A.1. *Under Condition 2, we have*

$$\left(\tilde{Z}_L(t_1, n_1), \tilde{Z}_L(t_2, n_2), \tilde{M}_L^{(l)}(t_1, n_1), \tilde{M}_L^{(r)}(t_1, n_1), \tilde{M}_L^{(l)}(t_2, n_2), \tilde{M}_L^{(r)}(t_2, n_2) \right)' \quad (\text{A.1})$$

asymptotically jointly normal and the covariance of

$$\left(\tilde{M}_L^{(l)}(t_1, n_1), \tilde{M}_L^{(r)}(t_1, n_1), \tilde{M}_L^{(l)}(t_2, n_2), \tilde{M}_L^{(r)}(t_2, n_2) \right) \quad (\text{A.2})$$

positive definite.

LEMMA A.2. *Under Condition 2, we have*

$$\lim_{L \rightarrow \infty} \frac{\text{Var}(\tilde{R}_L(t_1, n_1))}{\text{Var}(R_L(t_1, n_1))} = c_1, \quad \lim_{L \rightarrow \infty} \frac{\text{Var}(\tilde{R}_L(t_2, n_2))}{\text{Var}(R_L(t_2, n_2))} = c_2,$$

where c_1 and c_2 are constants.

From Lemma A.1, the conditional distribution of $(\tilde{Z}_L(t_1, n_1), \tilde{Z}_L(t_2, n_2))'$ given $(\tilde{M}_L^{(l)}(t_1, n_1), \tilde{M}_L^{(r)}(t_1, n_1), \tilde{M}_L^{(l)}(t_2, n_2), \tilde{M}_L^{(r)}(t_2, n_2))$ is bivariate normal as $L \rightarrow \infty$. Since the distribution of $(\tilde{Z}_L(t_1, n_1), \tilde{Z}_L(t_2, n_2))'$ conditioning on $(\tilde{M}_L^{(l)}(t_1, n_1) = 0, \tilde{M}_L^{(r)}(t_1, n_1) = 0, \tilde{M}_L^{(l)}(t_2, n_2) = 0, \tilde{M}_L^{(r)}(t_2, n_2) = 0)$ is equivalent to that conditioning on $\sum_{j \in n_{1,L}} A_{L,ij}^+(n_1) = k, \forall i \in n_{1,L}$ and $\sum_{j \in n_{2,L}} A_{L,ij}^+(n_2) = k, \forall i \in n_{2,L}$. Together with Lemma A.2 and

$$\mathbb{E}(\tilde{R}_L(t_1, n_1)) = \mathbb{E}(R_L(t_1, n_1)), \quad \mathbb{E}(\tilde{R}_L(t_2, n_2)) = \mathbb{E}(R_L(t_2, n_2)),$$

we have that $(Z_L(t_1, n_1), Z_L(t_2, n_2))'$ becomes bivariate normal as $L \rightarrow \infty$.

It is easy to show Lemma A.2 as

$$\begin{aligned} \lim_{L \rightarrow \infty} \frac{\text{Var}(\tilde{R}_L(t_1, n_1))}{\text{Var}(R_L(t_1, n_1))} &= \frac{2k + 2q_{1,\infty} + q_{2,\infty} - k^2}{k + 4u_1(1 - u_1)q_{1,\infty} + (1 - 2u_1)^2(q_{2,\infty} - k^2)}, \\ \lim_{L \rightarrow \infty} \frac{\text{Var}(\tilde{R}_L(t_2, n_2))}{\text{Var}(R_L(t_2, n_2))} &= \frac{2k + 2q_{1,\infty} + q_{2,\infty} - k^2}{k + 4u_2(1 - u_2)q_{1,\infty} + (1 - 2u_2)^2(q_{2,\infty} - k^2)}. \end{aligned}$$

The two limits are constants.

In the following, we prove Lemma A.1. It is easy to see that the covariance of (A.2) is positive definite under Condition 2. To show that (A.1) is jointly normal, we only need to show that $a_1\tilde{Z}_L(t_1, n_1) + a_2\tilde{Z}_L(t_2, n_2) + a_3\tilde{M}_L^{(l)}(t_1, n_1) + a_4\tilde{M}_L^{(r)}(t_1, n_1) + a_5\tilde{M}_L^{(l)}(t_2, n_2) + a_6\tilde{M}_L^{(r)}(t_2, n_2)$ is normal for any fixed a_1, \dots, a_6 . Let σ_0^2 be the variance of this summation. If $\sigma_0 = 0$, the quantity is degenerating. We show in the following the case when $\sigma_0 > 0$ that the quantity

$$\begin{aligned} W = \frac{1}{\sigma_0} &\left(a_1\tilde{Z}_L(t_1, n_1) + a_2\tilde{Z}_L(t_2, n_2) + a_3\tilde{M}_L^{(l)}(t_1, n_1) \right. \\ &\left. + a_4\tilde{M}_L^{(r)}(t_1, n_1) + a_5\tilde{M}_L^{(l)}(t_2, n_2) + a_6\tilde{M}_L^{(r)}(t_2, n_2) \right) \end{aligned}$$

is normal through Stein's method.

Consider sums of the form $W = \sum_{i \in \mathcal{I}} \xi_i$, where \mathcal{I} is an index set and ξ are random variables with $E(\xi_i) = 0$, and $E(W^2) = 1$. The following assumption restricts the dependence between $\{\xi_i : i \in \mathcal{I}\}$.

ASSUMPTION A.3. (*Chen and Shao, 2005, p. 17*) For each $i \in \mathcal{I}$ there exists $S_i \subset T_i \subset \mathcal{I}$ such that ξ_i is independent of $\xi_{S_i^c}$ and ξ_{S_i} is independent of $\xi_{T_i^c}$.

We will use the following specific form of Stein's method.

THEOREM A.4. (*Chen and Shao, 2005, Theorem 3.4*) Under Assumption A.3, we have

$$\sup_{h \in \text{Lip}(1)} |Eh(W) - Eh(Z)| \leq \delta$$

where $\text{Lip}(1) = \{h : \mathbb{R} \rightarrow \mathbb{R}, \|h'\| \leq 1\}$, Z has $\mathcal{N}(0, 1)$ distribution and

$$\delta = 2 \sum_{i \in \mathcal{I}} (E|\xi_i \eta_i \theta_i| + |E(\xi_i \eta_i)| E|\theta_i|) + \sum_{i \in \mathcal{I}} E|\xi_i \eta_i^2|$$

with $\eta_i = \sum_{j \in S_i} \xi_j$ and $\theta_i = \sum_{j \in T_i} \xi_j$, where S_i and T_i are defined in Assumption A.3.

Let

$$\sigma_1 = \sqrt{\text{Var}(\tilde{R}_L(t_1, n_1))}, \sigma_1^{(l)} = \sqrt{\text{Var}(\tilde{N}_L^{(l)}(t_1, n_1))}, \sigma_1^{(r)} = \sqrt{\text{Var}(\tilde{N}_L^{(r)}(t_1, n_1))},$$

$$\sigma_2 = \sqrt{\text{Var}(\tilde{R}_L(t_2, n_2))}, \sigma_2^{(l)} = \sqrt{\text{Var}(\tilde{N}_L^{(l)}(t_2, n_2))}, \sigma_2^{(r)} = \sqrt{\text{Var}(\tilde{N}_L^{(r)}(t_2, n_2))}.$$

Then $\sigma_1, \sigma_1^{(l)}, \sigma_1^{(r)}, \sigma_2, \sigma_2^{(l)}, \sigma_2^{(r)} \sim \mathcal{O}(L^{1/2})$

In the following, we write $A_{n_L, ij}^+$ as $A_{L, ij}^+(n)$ to avoid the cumbersome of the subscripts. Let

$$\xi_{ij,1} = \begin{cases} \frac{a_3}{\sigma_0 \sigma_1^{(l)}} \left(\tilde{A}_{L,ij}^+(n_1) - \frac{k}{L-1} \right) & i, j \in \{n_1 - L + 1, \dots, t_1\}, i \neq j, \\ \frac{2a_1 \sigma_1^{(l)} + a_3 \sigma_1}{\sigma_0 \sigma_1 \sigma_1^{(l)}} \left(\tilde{A}_{L,ij}^+(n_1) - \frac{k}{L-1} \right) & i \in \{n_1 - L + 1, \dots, t_1\}, \\ & j \in \{t_1 + 1, \dots, n_1\}, \\ \frac{2a_1 \sigma_1^{(r)} + a_4 \sigma_1}{\sigma_0 \sigma_1 \sigma_1^{(r)}} \left(\tilde{A}_{L,ij}^+(n_1) - \frac{k}{L-1} \right) & i \in \{t_1 + 1, \dots, n_1\}, \\ & j \in \{n_1 - L + 1, \dots, t_1\}, \\ \frac{a_4}{\sigma_0 \sigma_1^{(r)}} \left(\tilde{A}_{L,ij}^+(n_1) - \frac{k}{L-1} \right), & i, j \in \{n_1 - L + 1, \dots, t_1\}, i \neq j, \\ 0 & \text{otherwise,} \end{cases}$$

$$\xi_{ij,2} = \begin{cases} \frac{a_5}{\sigma_0 \sigma_2^{(l)}} \left(\tilde{A}_{L,ij}^+(n_2) - \frac{k}{L-1} \right) & i, j \in \{n_2 - L + 1, \dots, t_2\}, i \neq j, \\ \frac{2a_2 \sigma_2^{(l)} + a_5 \sigma_2}{\sigma_0 \sigma_2 \sigma_2^{(l)}} \left(\tilde{A}_{L,ij}^+(n_2) - \frac{k}{L-1} \right) & i \in \{n_2 - L + 1, \dots, t_2\}, \\ & j \in \{t_2 + 1, \dots, n_2\}, \\ \frac{2a_2 \sigma_2^{(r)} + a_6 \sigma_2}{\sigma_0 \sigma_2 \sigma_2^{(r)}} \left(\tilde{A}_{L,ij}^+(n_2) - \frac{k}{L-1} \right) & i \in \{t_2 + 1, \dots, n_2\}, \\ & j \in \{n_2 - L + 1, \dots, t_2\}, \\ \frac{a_6}{\sigma_0 \sigma_2^{(r)}} \left(\tilde{A}_{L,ij}^+(n_2) - \frac{k}{L-1} \right) & i, j \in \{n_2 - L + 1, \dots, t_2\}, i \neq j, \\ 0 & \text{otherwise,} \end{cases}$$

$$\xi_{ij} = \xi_{ij,1} + \xi_{ij,2}.$$

Then $W = \sum_{i,j} \xi_{ij}$ and ξ_{ij} is only dependent with $\{\xi_{ji}, \xi_{lj}, \forall l\}$. Adopting the same notations in Theorem A.4, we have

$$\eta_{ij} = \xi_{ij} + \xi_{ji} + \sum_l \xi_{lj},$$

$$\theta_{ij} = \xi_{ij} + \xi_{ji} + \sum_l (\xi_{lj} + \xi_{jl} + \xi_{li}).$$

Let

$$a = \max(|a_3|, |2a_1 + a_3|, |2a_1 + a_4|, |a_4|, |a_5|, |2a_2 + a_5|, |2a_2 + a_6|, |a_6|),$$

$$\sigma = \sigma_0 \times \min(\sigma_1, \sigma_1^{(l)}, \sigma_1^{(r)}, \sigma_2, \sigma_2^{(l)}, \sigma_2^{(r)}),$$

then $a = \mathcal{O}(1)$, $\sigma = \mathcal{O}(L^{1/2})$, and $|\xi_{ij}| \leq \frac{2ak}{\sigma}$.

Let $\tilde{N}_1(i) = \sum_{j \in n_{1,L}} \tilde{A}_{L,ij}^+(n_1)$, $\tilde{N}_2(i) = \sum_{j \in n_{2,L}} \tilde{A}_{L,ij}^+(n_2)$. Then, under Condition 1, we have

$$-k \frac{a}{\sigma} \leq \sum_l \xi_{jl,1} \leq \tilde{N}_1(j) \frac{a}{\sigma},$$

$$\begin{aligned}
 -k \frac{a}{\sigma} &\leq \sum_l \xi_{lj,1} \leq \mathbb{C} \frac{a}{\sigma}, \\
 -k \frac{a}{\sigma} &\leq \sum_l \xi_{jl,2} \leq \tilde{N}_2(j) \frac{a}{\sigma}, \\
 -k \frac{a}{\sigma} &\leq \sum_l \xi_{lj,2} \leq \mathbb{C} \frac{a}{\sigma}.
 \end{aligned}$$

So

$$\begin{aligned}
 \sum_l (\xi_{lj} + \xi_{jl} + \xi_{li}) &= \sum_l (\xi_{lj,1} + \xi_{jl,1} + \xi_{li,1} + \xi_{lj,2} + \xi_{jl,2} + \xi_{li,2}) \\
 &\in \left[-6k, \tilde{N}_1(j) + \tilde{N}_2(j) + 4\mathbb{C} \right] \times \frac{a}{\sigma}.
 \end{aligned}$$

Hence, $|\theta_{ij}| \leq (\tilde{N}_1(j) + \tilde{N}_2(j) + 4\mathbb{C} + 10k) \frac{a}{\sigma}$. Similarly $|\eta_{ij}| \leq (2\mathbb{C} + 6k) \frac{a}{\sigma}$.

Since

$$\begin{aligned}
 \left| \mathbb{E} \left(\left(A_{L,ij}^+(n_r) - \frac{k}{L-1} \right) \left(A_{L,i'j'}^+(n_{r'}) - \frac{k}{L-1} \right) \right) \right| &\leq \frac{2k}{L-1}, \\
 &\quad \forall i, j, i', j', \text{ and } r, r' \in \{1, 2\},
 \end{aligned}$$

we have $|\mathbb{E}(\xi_{ij}\xi_{lr})| \leq \frac{4a^2}{\sigma^2} \frac{2k}{L-1}$, so

$$\begin{aligned}
 &|\mathbb{E}(\xi_{ij}\eta_{ij})| \\
 &= |\mathbb{E}(\xi_{ij}(\xi_{ij} + \xi_{ji} + \sum_l \xi_{lj}))| \leq \frac{4a^2}{\sigma^2} \frac{2k}{L-1} (2 + \tilde{N}_1(j) + \tilde{N}_2(j)), \\
 &|\mathbb{E}(\xi_{ij}\eta_{ij}\theta_{ij})| \\
 &\leq |\mathbb{E}((\tilde{N}_1(j) + \tilde{N}_2(j) + 4\mathbb{C} + 10k) \frac{a}{\sigma} \frac{4a^2}{\sigma^2} \frac{2k}{L-1} (2 + \tilde{N}_1(j) + \tilde{N}_2(j)))| \\
 &= \frac{8a^3k}{\sigma^3(L-1)} (4\mathbb{C} + 12k + \mathbb{E}((\tilde{N}_1(j) + \tilde{N}_2(j))^2) + 2k(4\mathbb{C} + 10k)) \\
 &\leq \frac{8a^3k}{\sigma^3(L-1)} (4\mathbb{C} + 12k + 4(k^2 + k) + 2k(4\mathbb{C} + 10k)), \\
 &|\mathbb{E}(\xi_{ij}\eta_{ij}^2)| \\
 &\leq |\mathbb{E}((2\mathbb{C} + 6k) \frac{a}{\sigma} \frac{4a^2}{\sigma^2} \frac{2k}{L-1} (2 + \tilde{N}_1(j) + \tilde{N}_2(j)))| \\
 &= \frac{8a^3k}{\sigma^3(L-1)} (2\mathbb{C} + 6k)(2 + 2k).
 \end{aligned}$$

Hence

$$\delta \leq \frac{40a^3k}{\sigma^3(L-1)} (28k^2 + 16\mathbb{C} + 8k\mathbb{C}) L^2 = O(L^{-1/2}) \xrightarrow{L \rightarrow \infty} 0.$$

A.2. Proof of Theorem 4.4. Let $\rho_{L,(s,m)}(t,n) = \text{Cov}(Z_L(s,m), Z_L(t,n))$, then

$$\begin{aligned} \rho_{((m-s)/L, m/L)}^*((t-s)/L, (n-m)/L) &= \lim_{L \rightarrow \infty} \rho_{L,(s,m)}(t,n), \\ \left. \frac{\partial_+ \rho_{(u,w)}^*(\delta_1, 0)}{\partial \delta_1} \right|_{\delta_1=0} &= \lim_{L \rightarrow \infty} L \left. \frac{\partial \rho_{(s,m)}(t, m)}{\partial t} \right|_{t \searrow s}, \\ \left. \frac{\partial_- \rho_{(u,w)}^*(\delta_1, 0)}{\partial \delta_1} \right|_{\delta_1=0} &= \lim_{L \rightarrow \infty} L \left. \frac{\partial \rho_{(s,m)}(t, m)}{\partial t} \right|_{t \nearrow s}, \end{aligned}$$

and similar relations for the two directional partial derivatives with respect to δ_2 .

Without loss of generality, let $m \leq n$. Since we are only interested in these directional partial derivatives, we only need to figure out the covariance for two scenarios: (i) $s < t < m \leq n$, and (ii) $t < s < m \leq n$, under $(n-m) = o(L)$.

We have

$$\text{Cov}(Z_L(s, m), Z_L(t, n)) = \frac{\mathbb{E}(R_L(s, m)R_L(t, n)) - \mathbb{E}(R_L(s, m))\mathbb{E}(R_L(t, n))}{\sqrt{\text{Var}(R_L(s, m))\text{Var}(R_L(t, n))}}.$$

We know that

$$\mathbb{E}(R_L(t, n)) = \frac{4k(n-t)(L-n+t)}{L-1}, \quad (\text{A.3})$$

$$\begin{aligned} \text{Var}(R_L(t, n)) &= \frac{4(n-t)(L-n+t)}{L-1} \\ &\times \left(\frac{4(n-t-1)(L-n+t-1)}{(L-2)(L-3)} \left(p_{k,L} - q_{k,L} + \frac{(L-3)k^2}{L-1} \right) + (q_{k,L} + k - k^2) \right), \end{aligned} \quad (\text{A.4})$$

and similar equations for $\mathbb{E}(R_L(s, m))$ and $\text{Var}(R_L(s, m))$. So what we need to calculate is $\mathbb{E}(R_L(s, m)R_L(t, n))$ under the two scenarios.

(i) $s < t < m \leq n$

Notice that we can rewrite $R_L(s, m)$ and $R_L(t, n)$ to be

$$\begin{aligned} R_L(s, m) &= \sum_{i,j \in m_L} (A_{m_L,ij}^+ + A_{m_L,ji}^+) B_{ij}(s, m_L \cup n_L), \\ R_L(t, n) &= \sum_{i,j \in n_L} (A_{n_L,ij}^+ + A_{n_L,ji}^+) B_{ij}(t, m_L \cup n_L). \end{aligned}$$

For $i, j \in m_L \cap n_L$, we have

$$\mathbb{E}(B_{ij}(s, m_L \cup n_L) B_{ij}(t, m_L \cup n_L)) = \frac{2(L-(n-s))(m-t)}{(L-(n-m))(L-(n-m)-1)}. \quad (\text{A.5})$$

For $i \in m_L \cap n_L$, $j \in m_L$, $l \in n_L$, and $l \neq j$, we have

$$\begin{aligned} &\mathbb{E}(B_{ij}(s, m_L \cup n_L) B_{il}(t, m_L \cup n_L)) \\ &= \frac{(L-(n-s))[(m-t)(L-2) + (n-m)(m-s)]}{(L-(n-m))[(L-(n-m)-1)(L-2) + (n-m)(L-1)]} \end{aligned} \quad (\text{A.6})$$

$$+ \frac{(t-s)(L-(m-s))(n+m-2t)}{(L-(n-m))[(L-(n-m)-1)(L-2) + (n-m)(L-1)]}.$$

For $i, j \in m_L$, $l, r \in n_L$, $l \neq i, j$ and $r \neq i, j$, we have

$$\begin{aligned} & \mathbb{E}(B_{ij}(s, m_L \cup n_L) B_{lr}(t, m_L \cup n_L)) \\ &= \frac{4(L-(m-s))(L-(n-t)-1)[(n-t)(m-s)-(m-t)]}{L(L-1)(L-2)(L-3) + 2(n-m)(2L^2-6L+3) + 2(n-m)^2} \\ &+ \frac{4[(n-m)(m-t)(n-t-1)-(L-(n-s))(t-s)(n-t)]}{L(L-1)(L-2)(L-3) + 2(n-m)(2L^2-6L+3) + 2(n-m)^2}. \end{aligned} \quad (\text{A.7})$$

We denote the quantities in (A.5), (A.6) and (A.7) by $f_1(s, t)$, $f_2(s, t)$ and $f_3(s, t)$, respectively. Then

$$\begin{aligned} \mathbb{E}(R_L(s, m) R_L(t, n)) &= \mathbb{E}(\mathbb{E}(R_L(s, m) R_L(t, n) | \mathbf{Y})) \\ &= f_1(s, t) \mathbb{E} \left(\sum_{i, j \in m_L \cap n_L} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, ij}^+ + A_{n_L, ji}^+) \right) \\ &+ f_2(s, t) \mathbb{E} \left(\sum_{i \in m_L \cap n_L; j \in m_L, l \in n_L; l \neq j} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, il}^+ + A_{n_L, li}^+) \right) \\ &+ f_3(s, t) \mathbb{E} \left(\sum_{i, j \in m_L; l, r \in n_L; l \neq i, j; r \neq i, j} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, lr}^+ + A_{n_L, rl}^+) \right). \end{aligned}$$

Let

$$X_1 = \sum_{i, j \in m_L \cap n_L} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, ij}^+ + A_{n_L, ji}^+) \quad (\text{A.8})$$

$$= 2 \sum_{i, j \in m_L \cap n_L} (A_{m_L, ij}^+ A_{n_L, ij}^+ + A_{m_L, ij}^+ A_{n_L, ji}^+),$$

$$X_2 = \sum_{i \in m_L \cap n_L; j \in m_L, l \in n_L} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, il}^+ + A_{n_L, li}^+), \quad (\text{A.9})$$

$$\begin{aligned} &= (L-(n-m))k^2 + k \sum_{i \in m_L \cap n_L} D_{n_L}(i) + k \sum_{i \in m_L \cap n_L} D_{m_L}(i) \\ &+ \sum_{i \in m_L \cap n_L} D_{m_L}(i) D_{n_L}(i), \end{aligned}$$

$$X_3 = \sum_{i, j \in m_L; l, r \in n_L} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, lr}^+ + A_{n_L, rl}^+) = 4L^2 k^2,$$

where $D_{m_L}(i) = \sum_j A_{m_L, ji}^+$, $D_{n_L}(i) = \sum_j A_{n_L, ji}^+$.

Then

$$\sum_{i \in m_L \cap n_L; j \in m_L, l \in n_L; l \neq j} (A_{m_L, ij}^+ + A_{m_L, ji}^+) (A_{n_L, il}^+ + A_{n_L, li}^+) = X_2 - X_1,$$

$$\begin{aligned} & \sum_{i,j \in m_L; l,r \in n_L; l \neq i,j; r \neq i,j} (A_{m_L,ij}^+ + A_{m_L,ji}^+)(A_{n_L,lr}^+ + A_{n_L,rl}^+) \\ & = X_3 - 2X_1 - 4(X_2 - X_1) = X_3 + 2X_1 - 4X_2, \end{aligned}$$

and

$$\begin{aligned} \mathbb{E}(R_L(s, m)R_L(t, n)) &= (2f_1(s, t) - 4f_2(s, t) + 2f_3(s, t))\mathbb{E}(X_1) \\ &+ (4f_2(s, t) - 4f_3(s, t))\mathbb{E}(X_2) + 4L^2k^2f_3(s, t). \end{aligned} \quad (\text{A.10})$$

(ii) $t < s < m \leq n$

Following the same argument, we have

$$\begin{aligned} \mathbb{E}(R_L(s, m)R_L(t, n)) &= (2f_4(s, t) - 4f_5(s, t) + 2f_6(s, t))\mathbb{E}(X_1) \\ &+ (4f_5(s, t) - 4f_6(s, t))\mathbb{E}(X_2) + 4L^2k^2f_6(s, t), \end{aligned} \quad (\text{A.11})$$

where

$$\begin{aligned} f_4(s, t) &= \frac{2(L - (n - t))(m - s)}{(L - (n - m))(L - (n - m) - 1)}, \\ f_5(s, t) &= \frac{(L - (n - t))(m - s)(L + n - m + 2s - 2t - 2)}{(L - (n - m))((L - (n - m) - 1)(L - 2) + (n - m)(L - 1))}, \\ f_6(s, t) &= \frac{4(L - (n - t))(m - s)[(n - t - 1)(L - (m - s) - 1) - (s - t)]}{L(L - 1)(L - 2)(L - 3) + 2(n - m)(2L^2 - 6L + 3) + 2(n - m)^2}. \end{aligned}$$

So for both scenarios, the problem boils down to calculate $\mathbb{E}(X_1)$ and $\mathbb{E}(X_2)$. It is easy to have that

$$\mathbb{E}\left(\sum_{i \in m_L \cap n_L} D_{n_L}(i)\right) = \mathbb{E}\left(\sum_{i \in m_L \cap n_L} D_{m_L}(i)\right) = k(L - (n - m)). \quad (\text{A.12})$$

In the following, we calculate the remaining three quantities:

$$\mathbb{E}\left(\sum_{i,j \in m_L \cap n_L} A_{m_L,ij}^+ A_{n_L,ij}^+\right), \quad (\text{A.13})$$

$$\mathbb{E}\left(\sum_{i,j \in m_L \cap n_L} A_{m_L,ij}^+ A_{n_L,ji}^+\right), \quad (\text{A.14})$$

$$\mathbb{E}\left(\sum_{i \in m_L \cap n_L} D_{m_L}(i) D_{n_L}(i)\right). \quad (\text{A.15})$$

We calculate them under $(n - m) = o(L)$.

For (A.13), we have

$$\mathbb{E}\left(\sum_{i,j \in m_L \cap n_L} A_{m_L,ij}^+ A_{n_L,ij}^+\right)$$

$$= (L - (n - m))(L - (n - m) - 1)P(A_{m_L,ij}^+ = 1, A_{n_L,ij}^+ = 1).$$

For $i, j \in m_L \cap n_L$, $i \neq j$, when $k = 1$,

$$P(A_{m_L,ij}^+ = 1, A_{n_L,ij}^+ = 1) = P(A_{m_L \cup n_L,ij}^+ = 1) = \frac{1}{L + n - m - 1}.$$

When $k > 1$,

$$\begin{aligned} & P(A_{m_L,ij}^+ = 1, A_{n_L,ij}^+ = 1) \\ &= P(A_{m_L \cup n_L,ij}^+ = 1) + P(A_{m_L,ij}^+ = 1, A_{n_L,ij}^+ = 1, A_{m_L \cup n_L,ij}^+ = 0) \\ &= \frac{k}{L + n - m - 1} + O\left(\frac{(n - m)^2}{L^3}\right). \end{aligned}$$

The event $\{A_{m_L,ij}^+ = 1, A_{n_L,ij}^+ = 1, A_{m_L \cup n_L,ij}^+ = 0\}$ implies that there is at least one observation in $\{m - L + 1, \dots, n - L\}$ and another observation in $\{m + 1, \dots, n\}$ whose distance to \mathbf{Y}_i is smaller than the distance between \mathbf{Y}_i and \mathbf{Y}_j . The order of its probability follows by considering the possible locations of the first k NNs of Y_i among all observations in $m_L \cup n_L$. So

$$\begin{aligned} & \mathbb{E} \left(\sum_{i,j \in m_L \cap n_L} A_{m_L,ij}^+ A_{n_L,ij}^+ \right) \\ &= \frac{k(L - (n - m))(L - (n - m) - 1)}{L + n - m - 1} + (k - 1) O\left(\frac{(n - m)^2}{L}\right) \\ &= k(L - 3(n - m)) + O\left(\frac{(n - m)^2}{L}\right). \end{aligned} \tag{A.16}$$

For (A.14), notice that, for $i, j \in m_L \cap n_L$, $i \neq j$,

$$\begin{aligned} & P(A_{m_L,ij}^+ = 1, A_{n_L,ji}^+ = 1) \\ &= P(A_{m_L \cup n_L,ij}^+ = 1, A_{m_L \cup n_L,ji}^+ = 1) \\ &+ P(A_{n_L,ji}^+ = 1, A_{m_L \cup n_L,ij}^+ = 1, A_{m_L \cup n_L,ji}^+ = 0) \\ &+ P(A_{m_L,ij}^+ = 1, A_{m_L \cup n_L,ij}^+ = 0, A_{m_L \cup n_L,ji}^+ = 1) \\ &+ P(A_{m_L,ij}^+ = 1, A_{n_L,ji}^+ = 1, A_{m_L \cup n_L,ij}^+ = 0, A_{m_L \cup n_L,ji}^+ = 0) \\ &= \frac{2p_{k,L}}{L - 1} - \frac{q_{1,L+n-m}^{(k)}}{L + n - m - 1} - \frac{2(n - m) \sum_{r=1}^k p_{k,L}(k, r)}{(L - 1)(L + n - m - 2)} + O\left(\frac{(n - m)^2}{L^3}\right). \end{aligned}$$

The last step can be obtained by considering all possible locations of the first k NNs of \mathbf{Y}_i among all observations in $m_L \cup n_L$, and all possible locations of the first k NNs of \mathbf{Y}_j among all observations in $m_L \cup n_L$. Then, we have, after simplification,

$$\mathbb{E} \left(\sum_{i,j \in m_L \cap n_L} A_{m_L,ij}^+ A_{n_L,ji}^+ \right) = L(2p_{k,L} - p_{k,L+n-m}) \tag{A.17}$$

$$-(n-m) \left(4p_{k,L} - 3p_{k,L+n-m} + 2 \sum_{r=1}^k p_{k,L}(k,r) \right) + O\left(\frac{(n-m)^2}{L}\right).$$

For (A.15), we have

$$\begin{aligned} \mathbb{E} \left(\sum_{i \in m_L \cap n_L} D_{m_L}(i) D_{n_L}(i) \right) &= \mathbb{E} \left(\sum_{i \in m_L \cap n_L; j \in m_L; l \in n_L} A_{m_L,ji}^+ A_{n_L,li}^+ \right) \\ &= \mathbb{E} \left(\sum_{i,j \in m_L \cap n_L} A_{m_L,ji}^+ A_{n_L,ji}^+ \right) + \mathbb{E} \left(\sum_{i \in m_L \cap n_L; j \in m_L; l \in n_L; l \neq j} A_{m_L,ji}^+ A_{n_L,li}^+ \right). \end{aligned}$$

The first part of the summation is (A.13). For the second part, notice that, for $i \in m_L \cap n_L$, $j \in m_L$, $l \in n_L$, $l \neq j$,

$$\begin{aligned} &\mathbb{P}(A_{m_L,ji}^+ = 1, A_{n_L,li}^+ = 1) \\ &= \mathbb{P}(A_{m_L \cup n_L,ji}^+ = 1, A_{m_L \cup n_L,li}^+ = 1) \\ &\quad + \mathbb{P}(A_{m_L,ji}^+ = 1, A_{m_L \cup n_L,ji}^+ = 0, A_{m_L \cup n_L,li}^+ = 1) \\ &\quad + \mathbb{P}(A_{n_L,li}^+ = 1, A_{m_L \cup n_L,ji}^+ = 1, A_{m_L \cup n_L,li}^+ = 0) \\ &\quad + \mathbb{P}(A_{m_L,ji}^+ = 1, A_{n_L,li}^+ = 1, A_{m_L \cup n_L,ji}^+ = 0, A_{m_L \cup n_L,li}^+ = 0) \\ &= \frac{2q_{k,L}}{(L-1)(L-2)} - \frac{q_{k,L+n-m}}{(L+n-m-1)(L+n-m-2)} \\ &\quad - \frac{2(n-m) \sum_{r=1}^k q_L(k,r)}{(L-1)(L-2)(L+n-m-2)} + O\left(\frac{(n-m)^2}{L^4}\right). \end{aligned}$$

The last step can be obtained by considering all possible locations of the first k NNs of \mathbf{Y}_j among all observations in $m_L \cup n_L$, and all possible locations of the first k NNs of \mathbf{Y}_l among all observations in $m_L \cup n_L$. Then, we have, after simplification,

$$\begin{aligned} \mathbb{E} \left(\sum_{i \in m_L \cap n_L} D_{m_L}(i) D_{n_L}(i) \right) &= L(k + 2q_{k,L} - q_{k,L+n-m}) \quad (\text{A.18}) \\ &+ (n-m) \left(3q_{k,L+n-m} - 2q_{k,L} - 3k - 2 \sum_{r=1}^k q_L(k,r) \right) + O\left(\frac{(n-m)^2}{L}\right). \end{aligned}$$

Plugging (A.12), (A.16), (A.17) and (A.18) into (A.10) and (A.11), we get an analytic expression of the covariance between $Z_L(s, m)$ and $Z_L(t, n)$. Taking partial derivatives over t and n , respectively, and then taking the limit, after some tedious calculations, we get Theorem 4.4.

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